

Supporting Information

Access to C4-arylated benzoxazoles from 2-amidophenol through C-H activation

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National Institute of Technology Rourkela, Odisha-769008, India

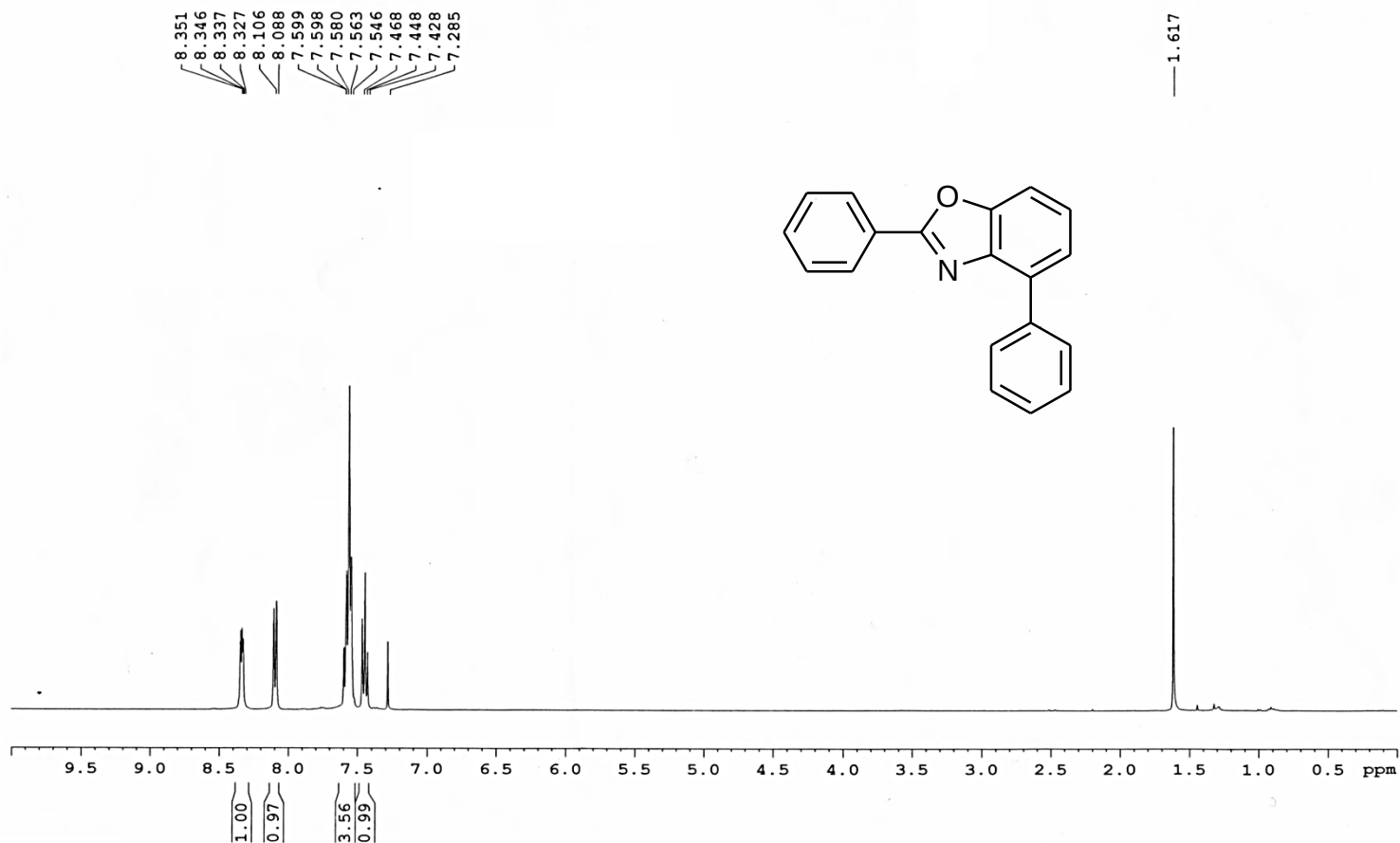
Contents

^1H and ^{13}C NMR spectra

¹H NMR of 2, 4-biphenyl benzo[d]oxazole (3aa)

¹H of NP-KS-STD

6.8.2019

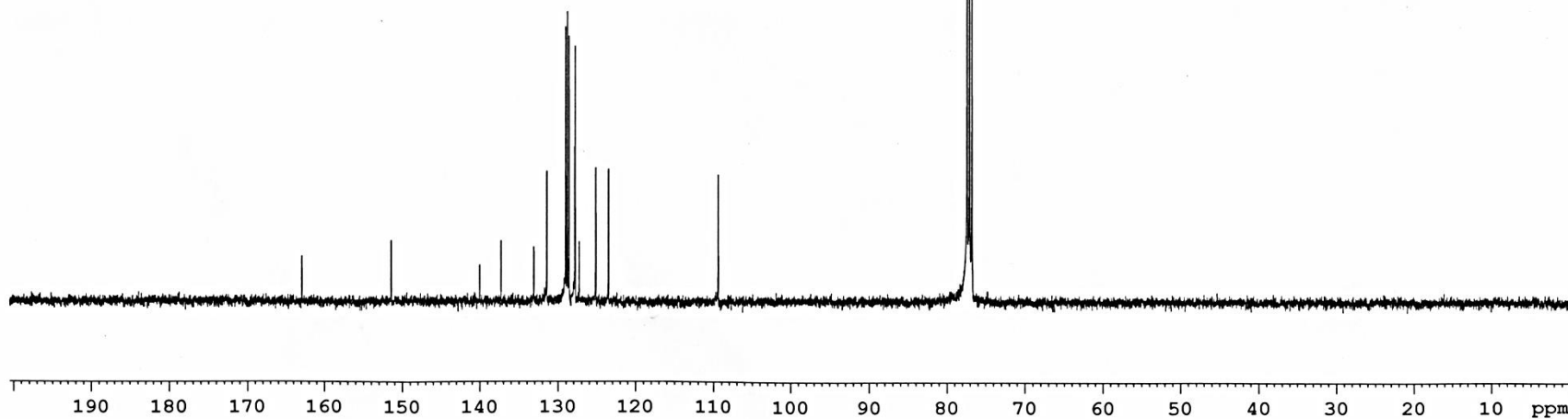
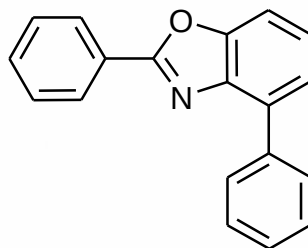


^{13}C NMR of 2,4-biphenyl benzo[d]oxazole (3aa)

^{13}C of NP-KS-STD

8.8.2019

— 162.90
— 151.41
139.99
137.28
133.10
131.44
129.05
128.82
128.60
127.85
127.80
127.29
125.14
123.50
— 109.41
77.35
77.04
76.72

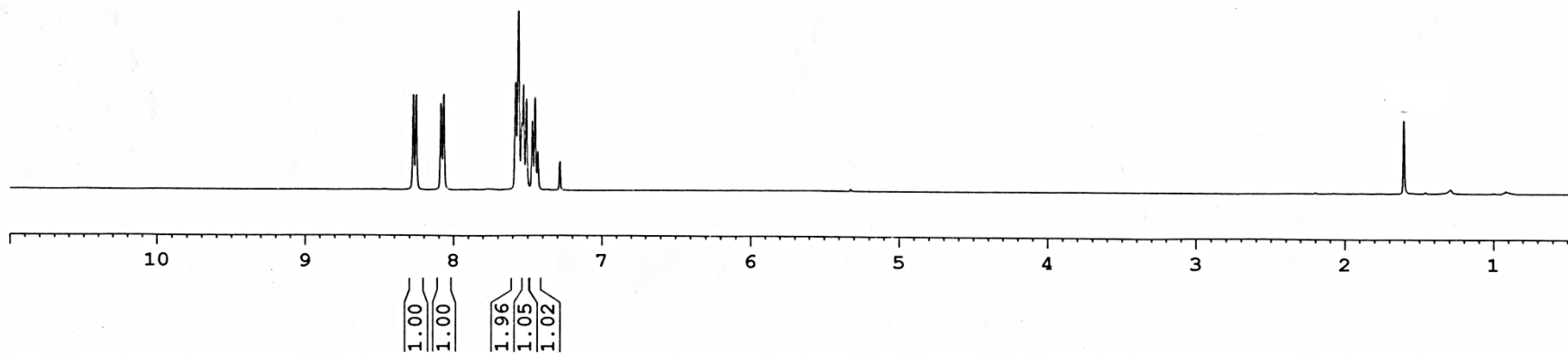
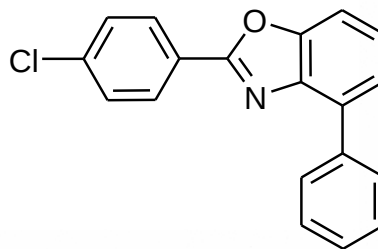


¹H NMR of 2-(4-chlorophenyl)-4-phenylbenzo[d]oxazole (3ba)

¹H of NP-KS-698

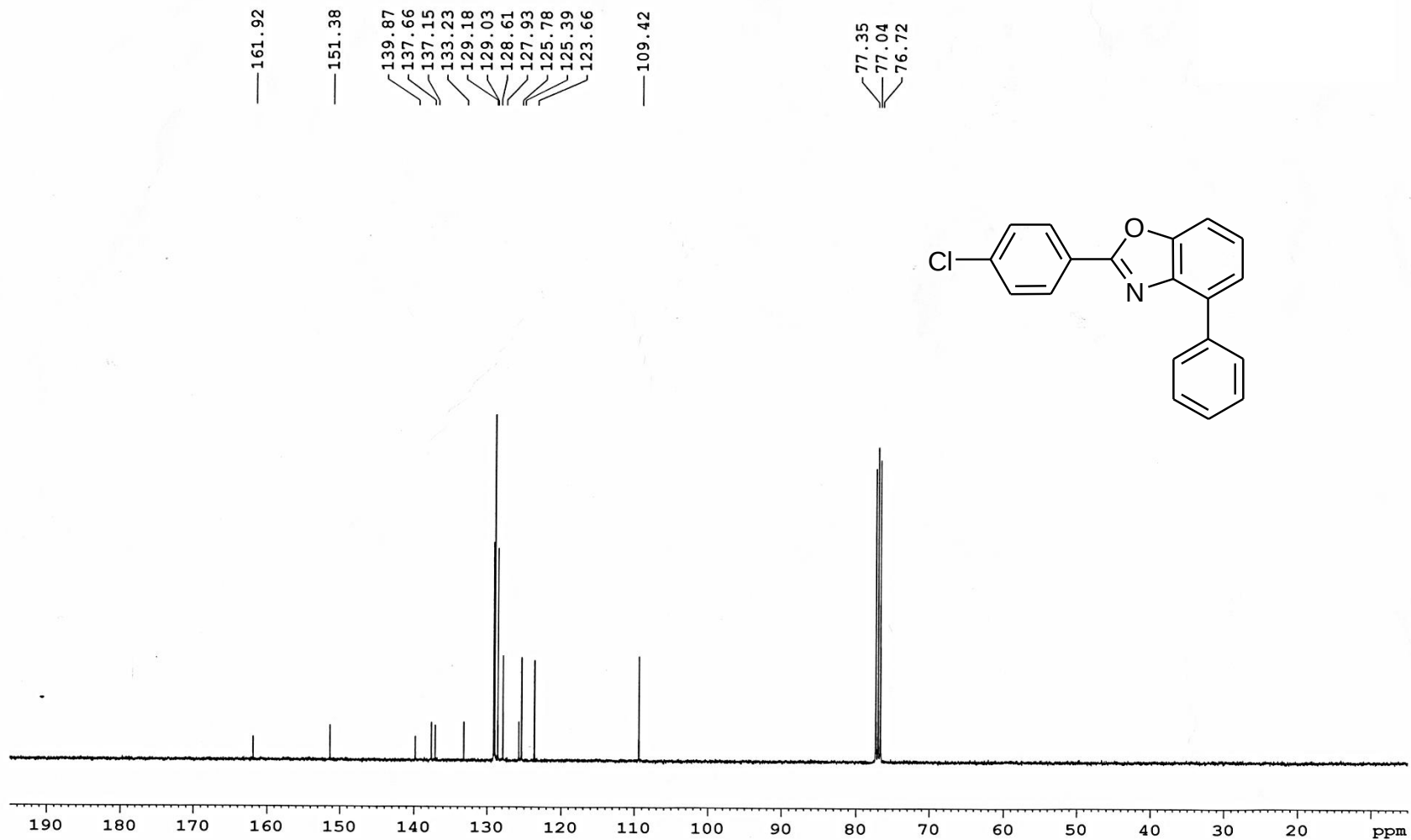
8.273
8.252
8.086
8.066
7.584
7.563
7.541
7.531
7.510
7.472
7.453
7.433
7.284

— 1.604



^{13}C NMR of 2-(4-chlorophenyl)-4-phenylbenzo[d]oxazole (3ba)

^1H of NP-KS-698



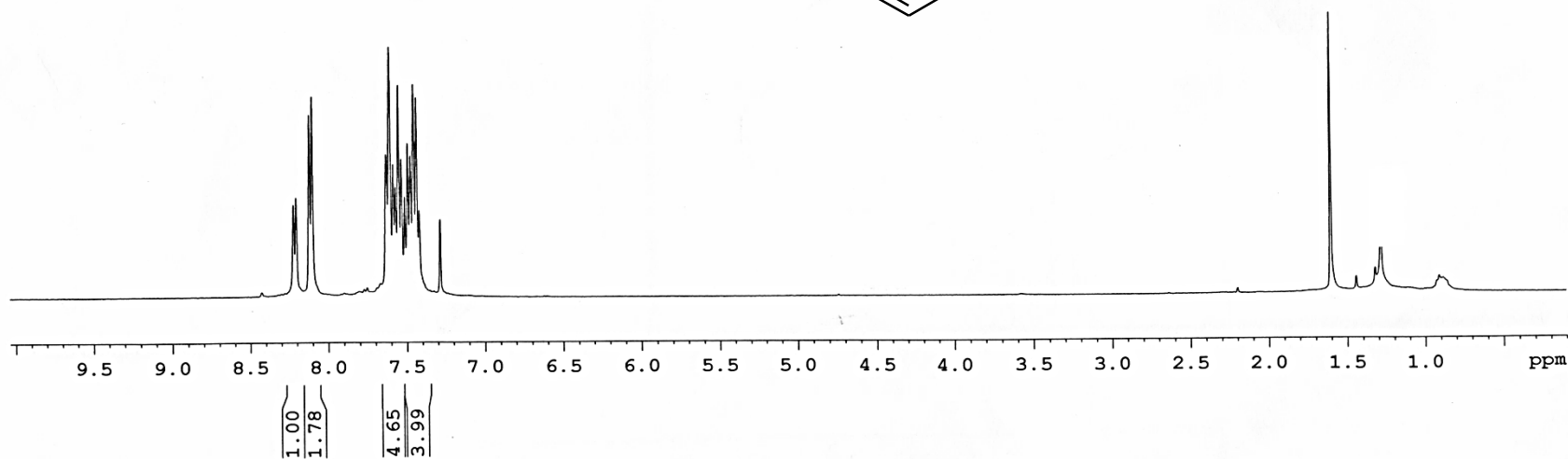
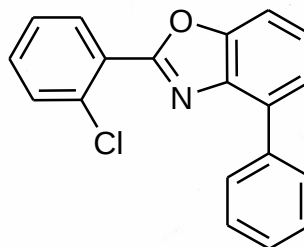
^1H NMR of 2-(2-chlorophenyl)-4-phenylbenzo[d]oxazole (3ca)

^1H of NP-KS-746

14.8.2019

8.223
8.204
8.121
8.102
7.631
7.611
7.587
7.571
7.552
7.534
7.513
7.495
7.477
7.457
7.438
7.420
7.284

— 1.602
— 1.286



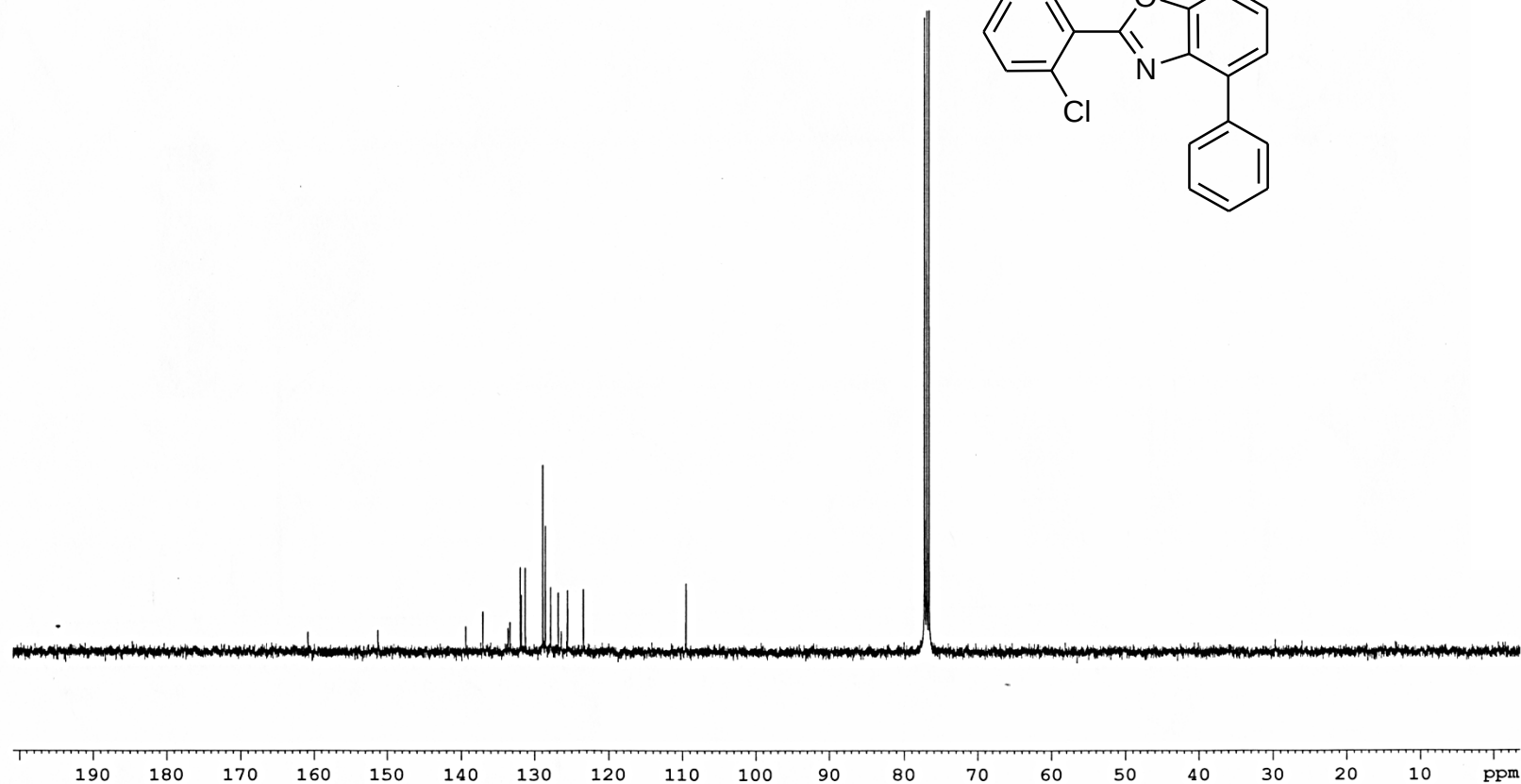
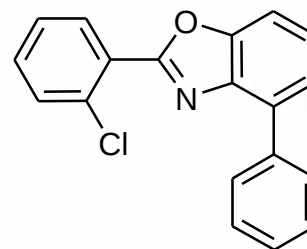
^{13}C NMR of 2-(2-chlorophenyl)-4-phenylbenzo[d]oxazole (3ca)

13C of NP-KS-746

14.8.2019

160.92
151.31
139.45
137.10
133.67
133.41
132.00
131.84
131.32
128.97
128.61
127.89
126.86
126.45
125.61
123.48
109.58

77.34
77.02
76.70

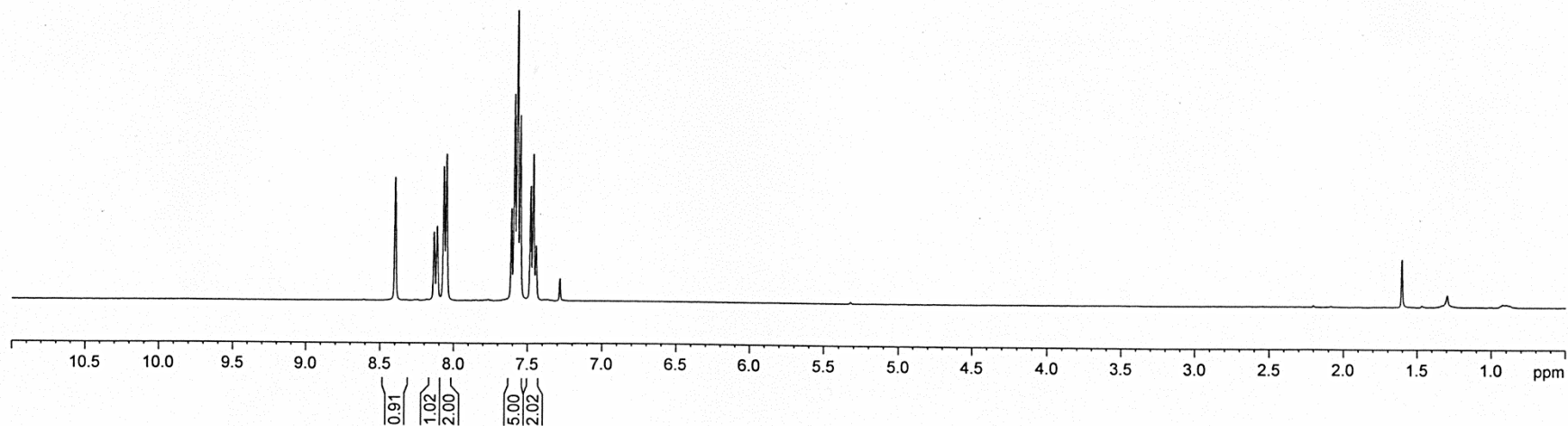
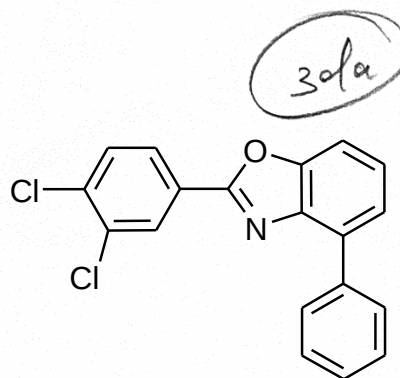


^1H NMR of 2-(3, 4 - dichlorophenyl)-4-phenylbenzo[d]oxazole (3da)

^1H of NP-KS-702

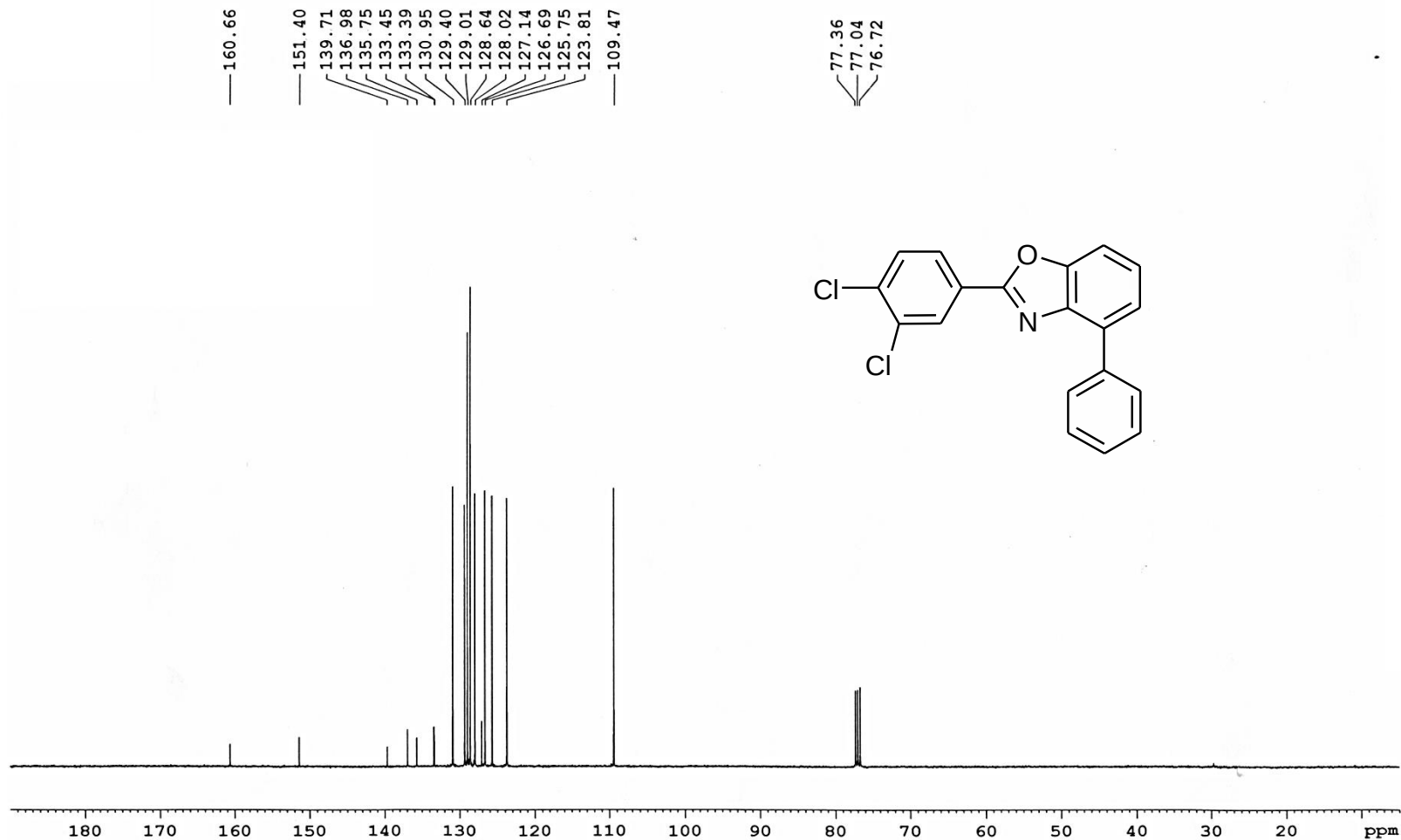
8.400
8.136
8.115
8.071
8.051
7.610
7.590
7.571
7.551
7.481
7.463
7.444
7.284

1.605

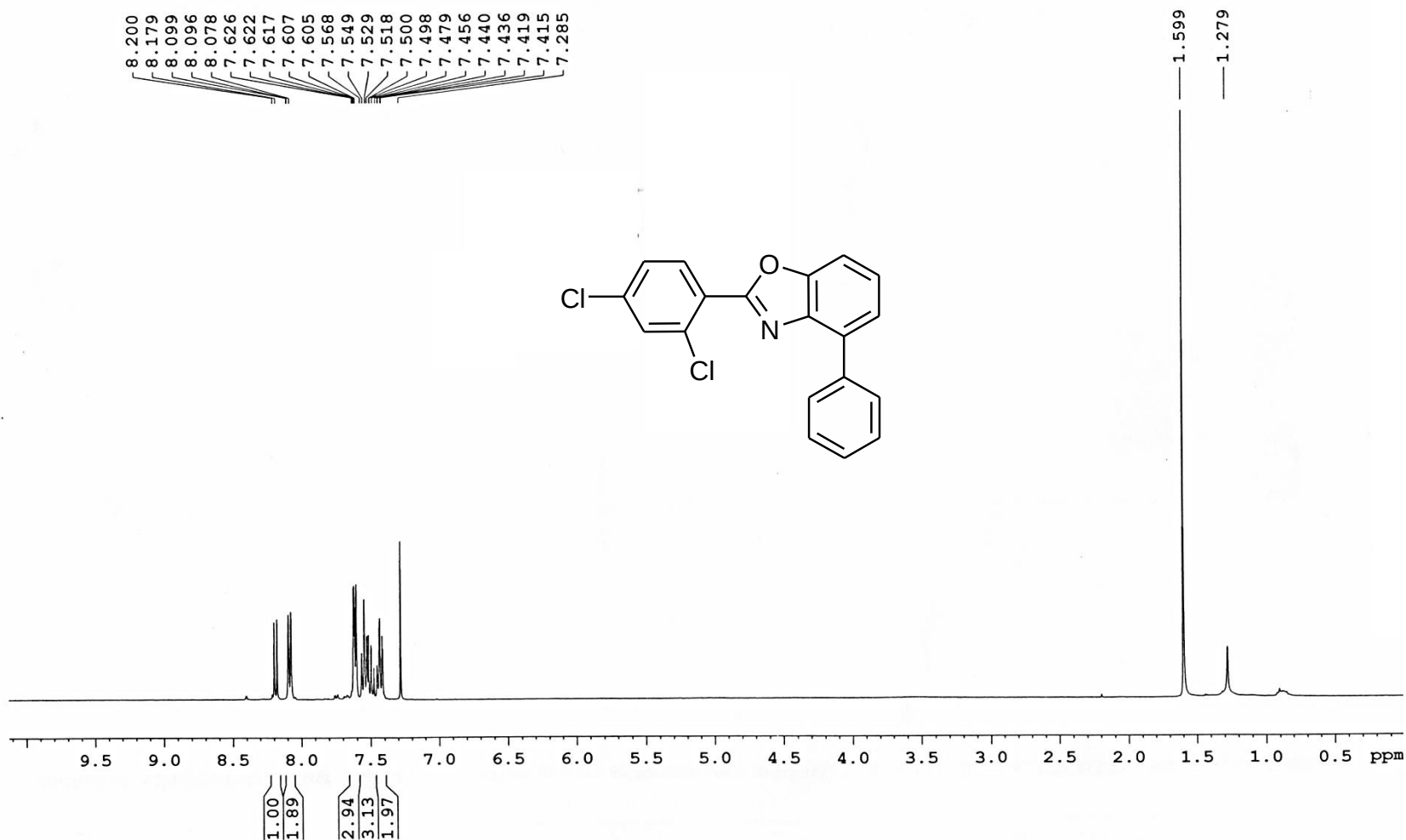


^{13}C NMR of 2-(3, 4 - dichlorophenyl)-4-phenylbenzo[d]oxazole (3da)

^{13}C of NP-KS-702

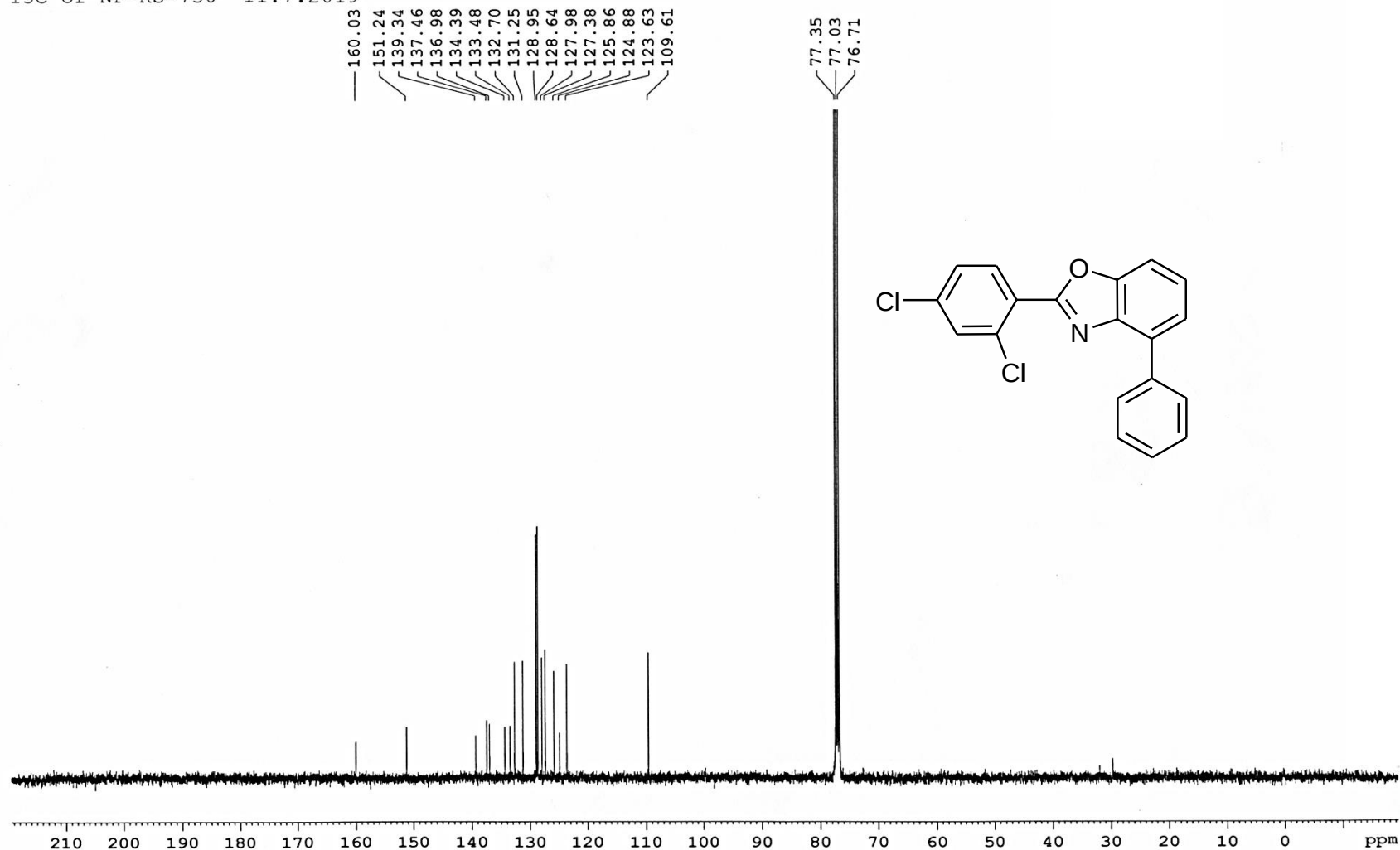


^1H NMR of 2-(2, 4 - dichlorophenyl)-4-phenylbenzo[d]oxazole (3ea)



¹³C NMR of 2-(2, 4 - dichlorophenyl)-4-phenylbenzo[d]oxazole (3ea)

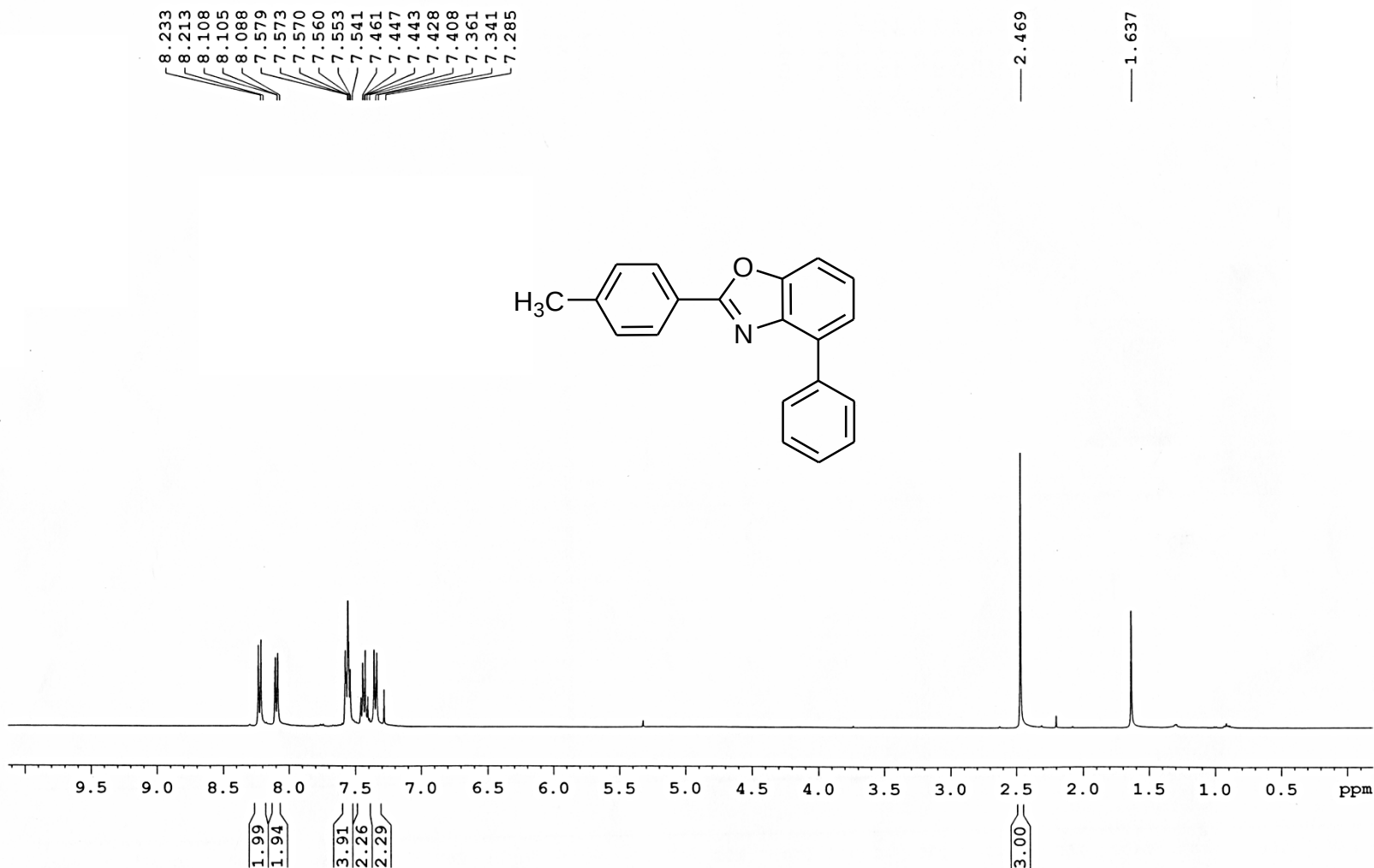
¹³C of NP-KS-730 11.7.2019



¹H NMR of 4-phenyl -2- p-tolylbenz[d]oxazole(3fa)

¹H of NP-KS-744

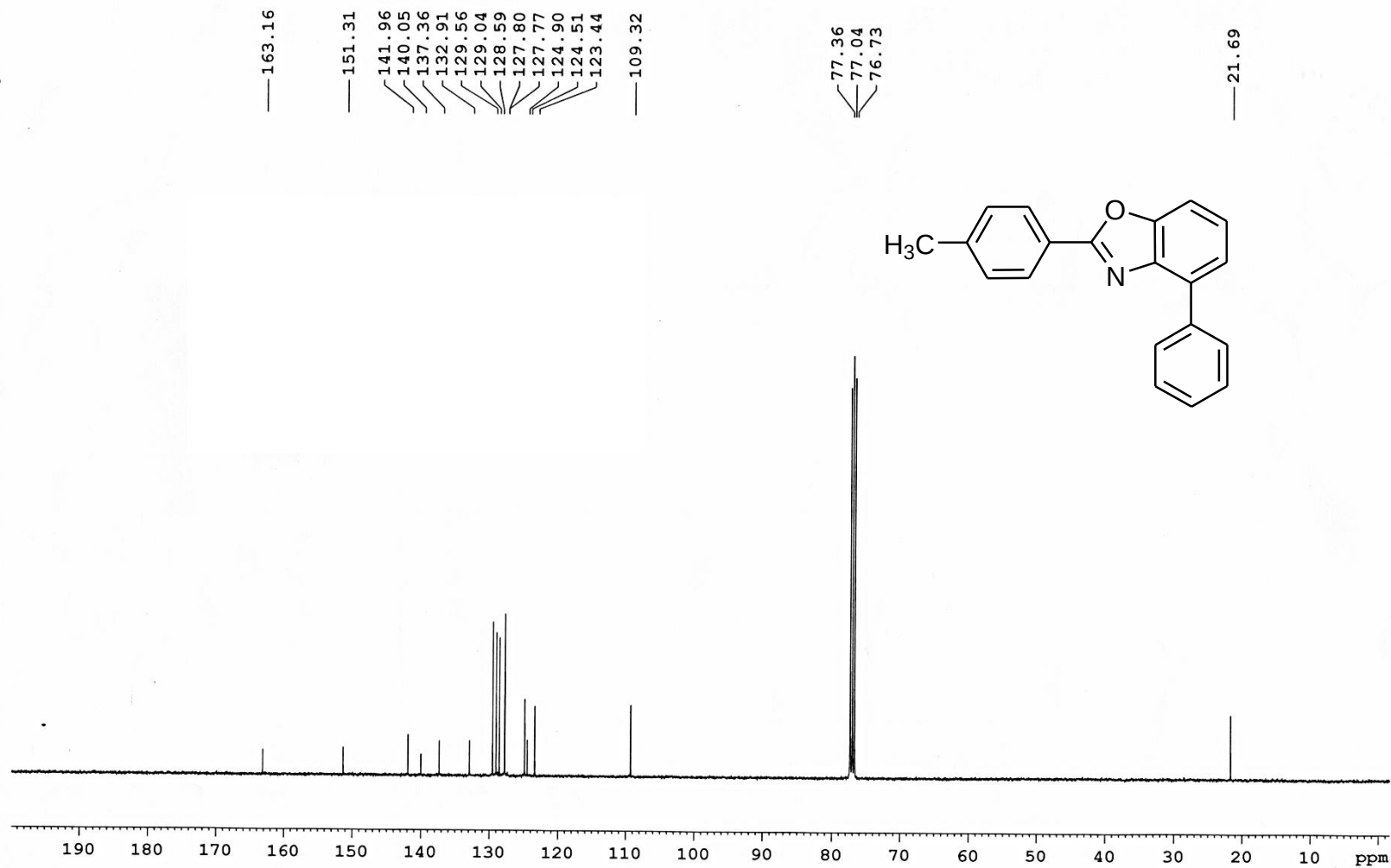
5.8.2019



¹³C NMR of 4-phenyl -2- p-tolylbenz[d]oxazole(3fa)

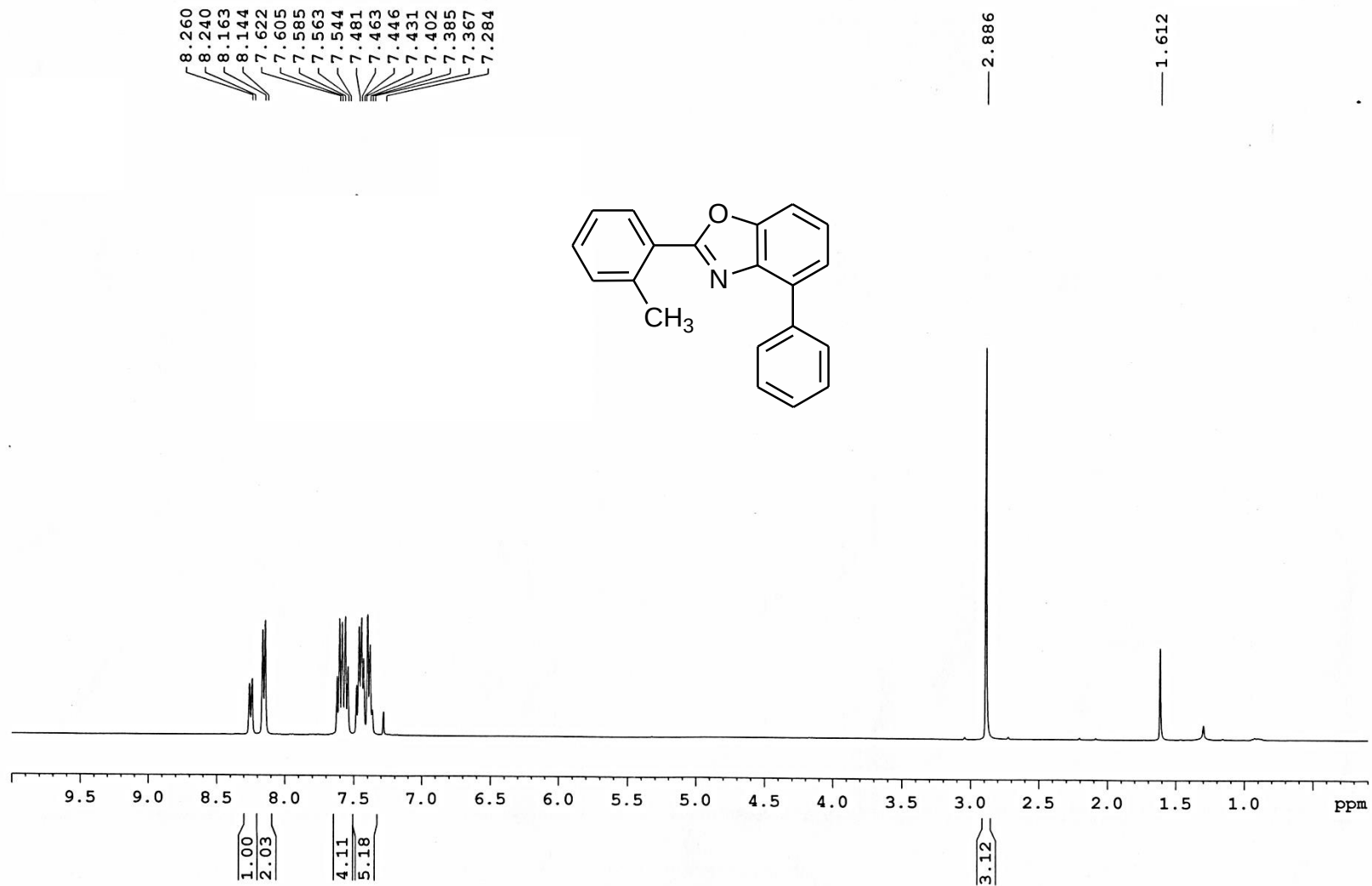
¹³DC of NP-KS-744

5.8.2019



¹H NMR of 4-phenyl -2- o-tolylbenz[d]oxazole (3ga)

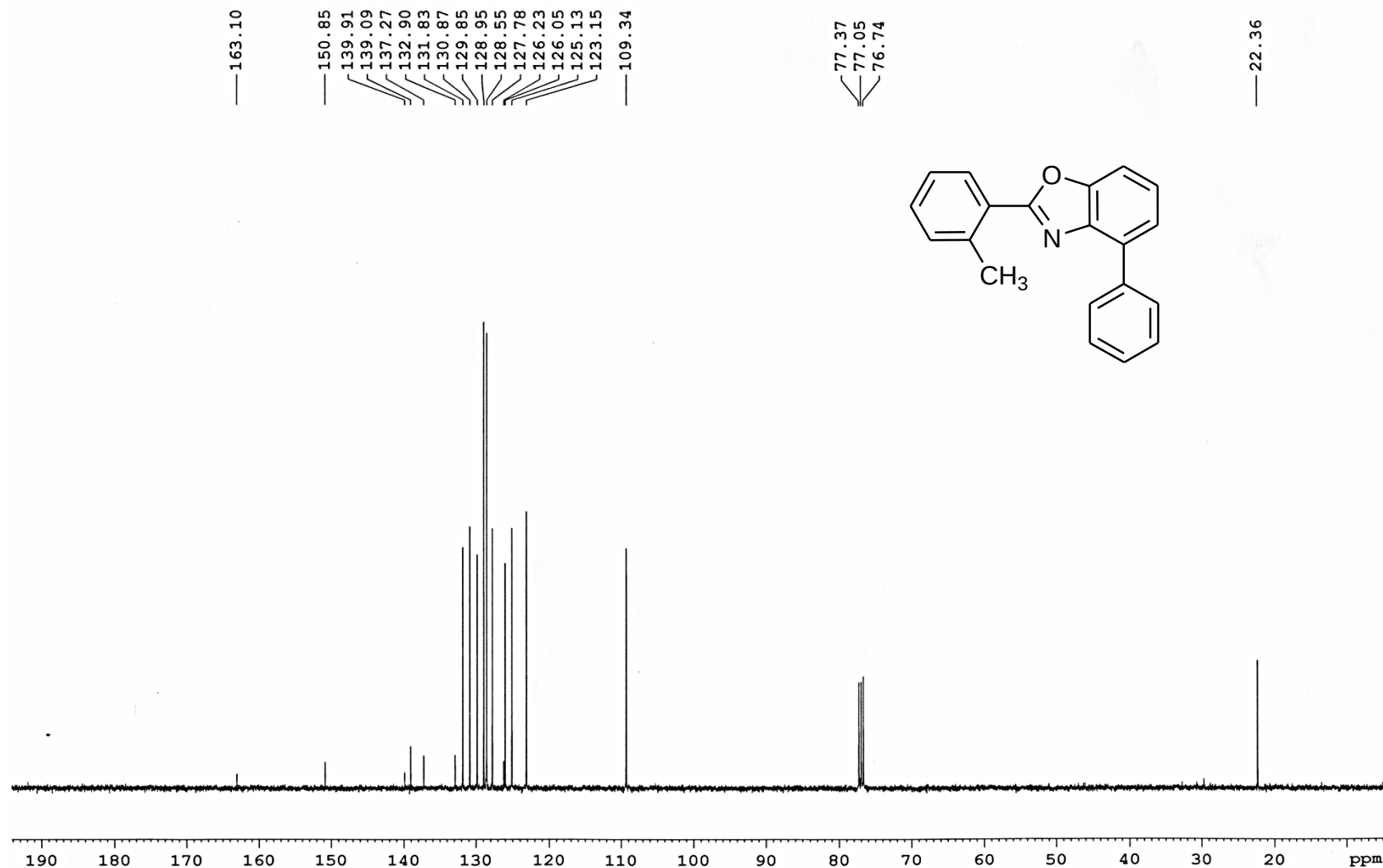
1h of NP-KS-719(o-me) 7.6.2019



¹³C NMR of 4-phenyl -2- o-tolylbenz[d]oxazole (3ga)

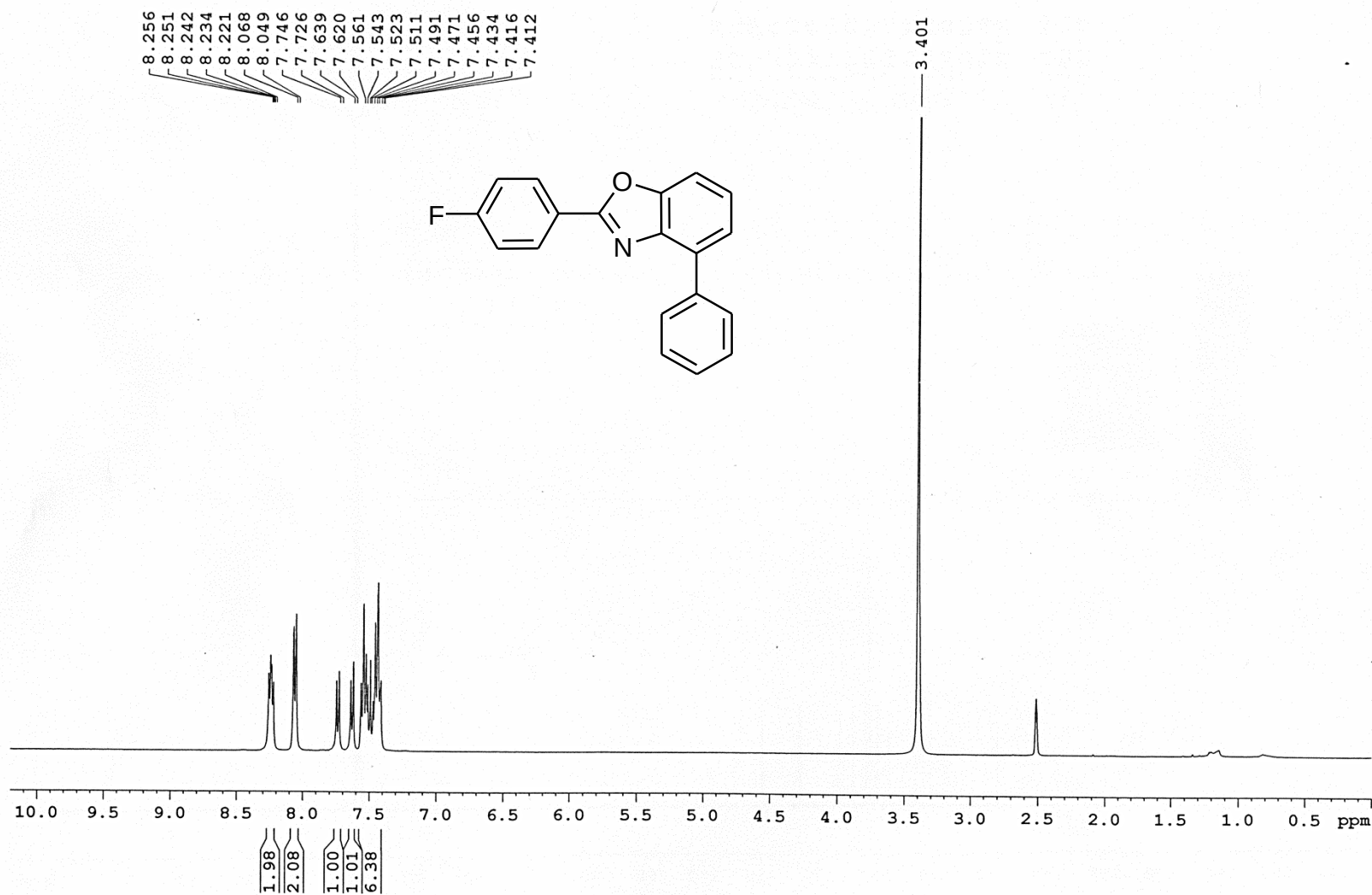
13c of NP-KS-719(o-me)

7.6.2019



¹H NMR of 2-(4-fluorophenyl)-4-phenylbenzo[d]oxazole (3ha)

¹H of NP_KS-aryl F 31.1.2020 (DMSO-d₆)

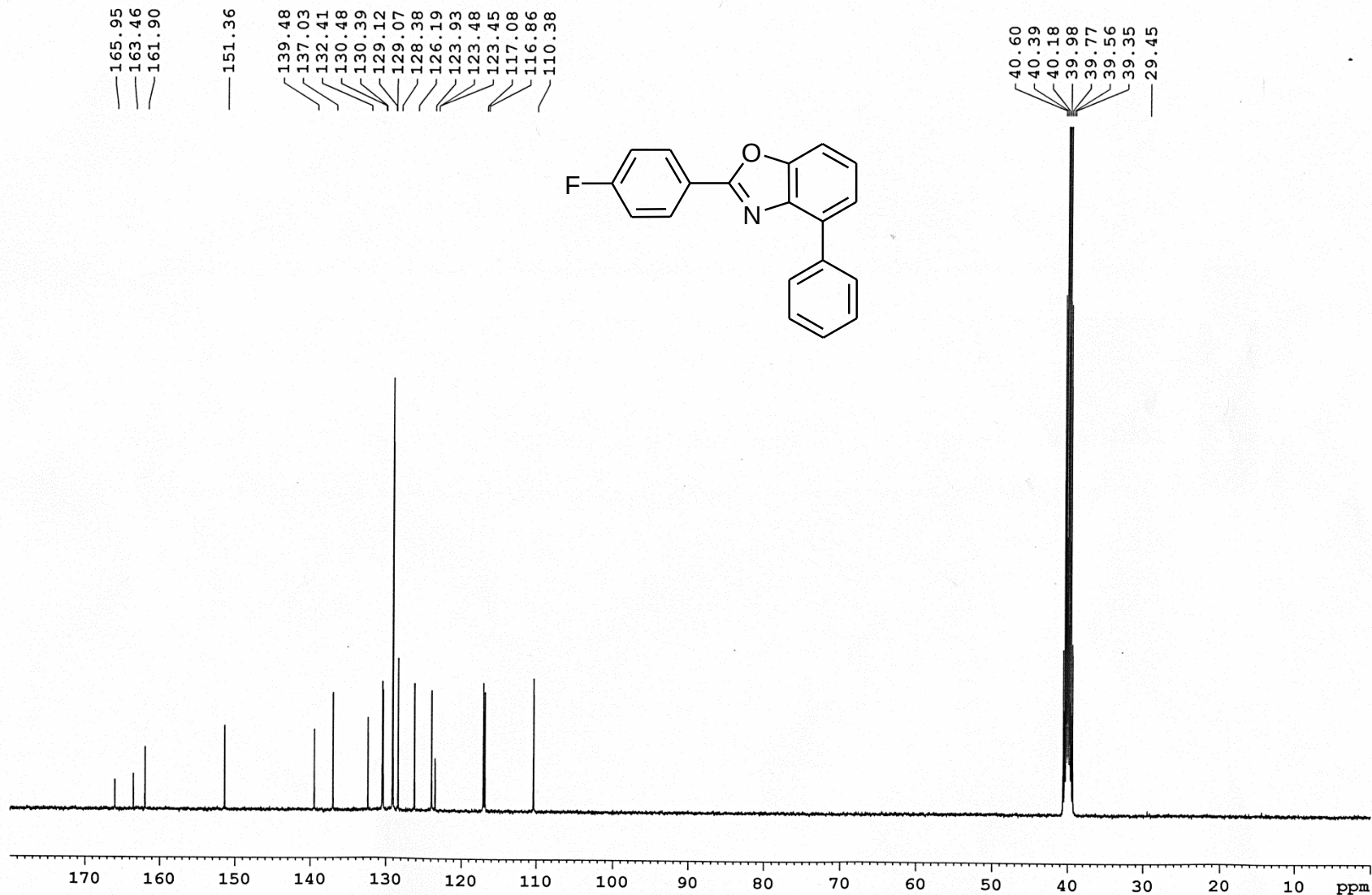


^{13}C NMR of 2-(4-fluorophenyl)-4-phenylbenzo[d]oxazole (3ha)

^{13}C of NP_KS-aryl F

31.1.2020

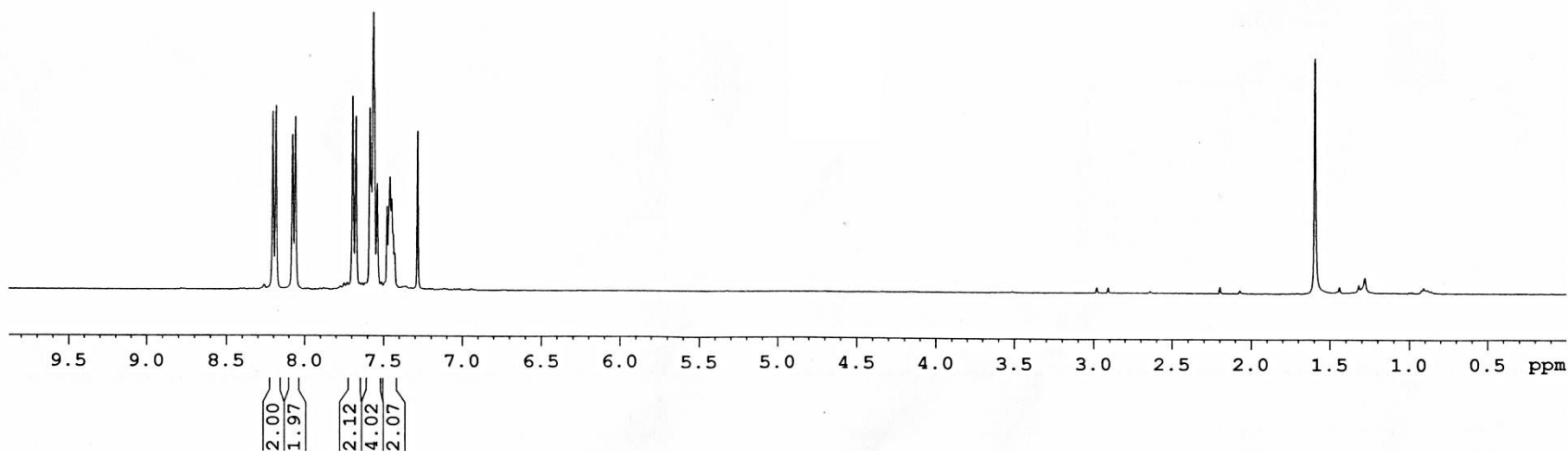
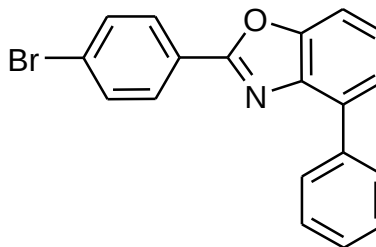
(DMSO- d_6)



^1H NMR of 2-(4-bromophenyl)-4-phenylbenzo[d]oxazole (3ia)

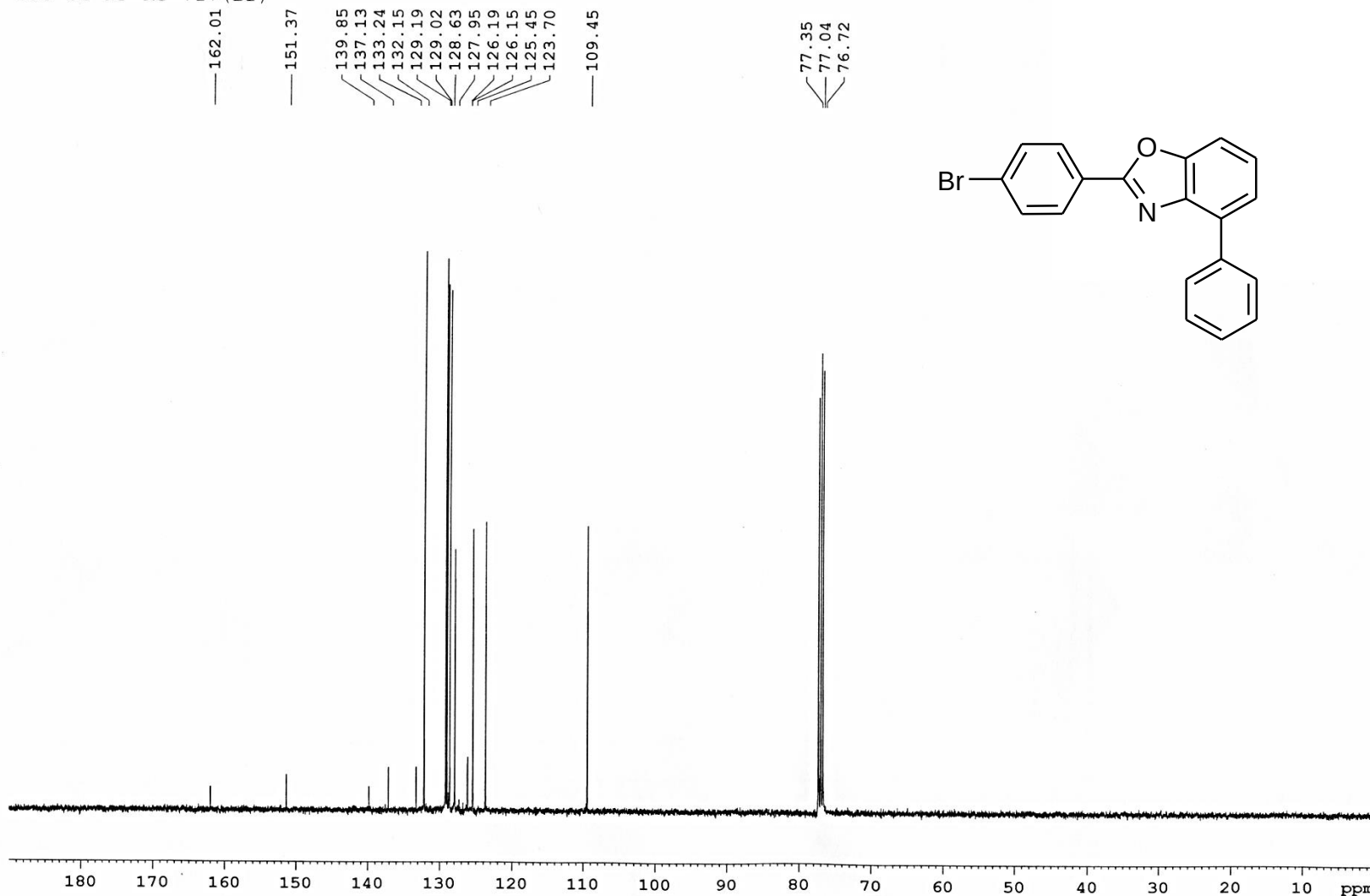
^1H of NP-KS-717 (Br) 31.5.2019

8.204
8.183
8.078
8.059
7.694
7.673
7.586
7.577
7.566
7.559
7.539
7.477
7.459
7.448
7.429
7.285



^{13}C NMR of 2-(4-bromophenyl)-4-phenylbenzo[d]oxazole (3ia)

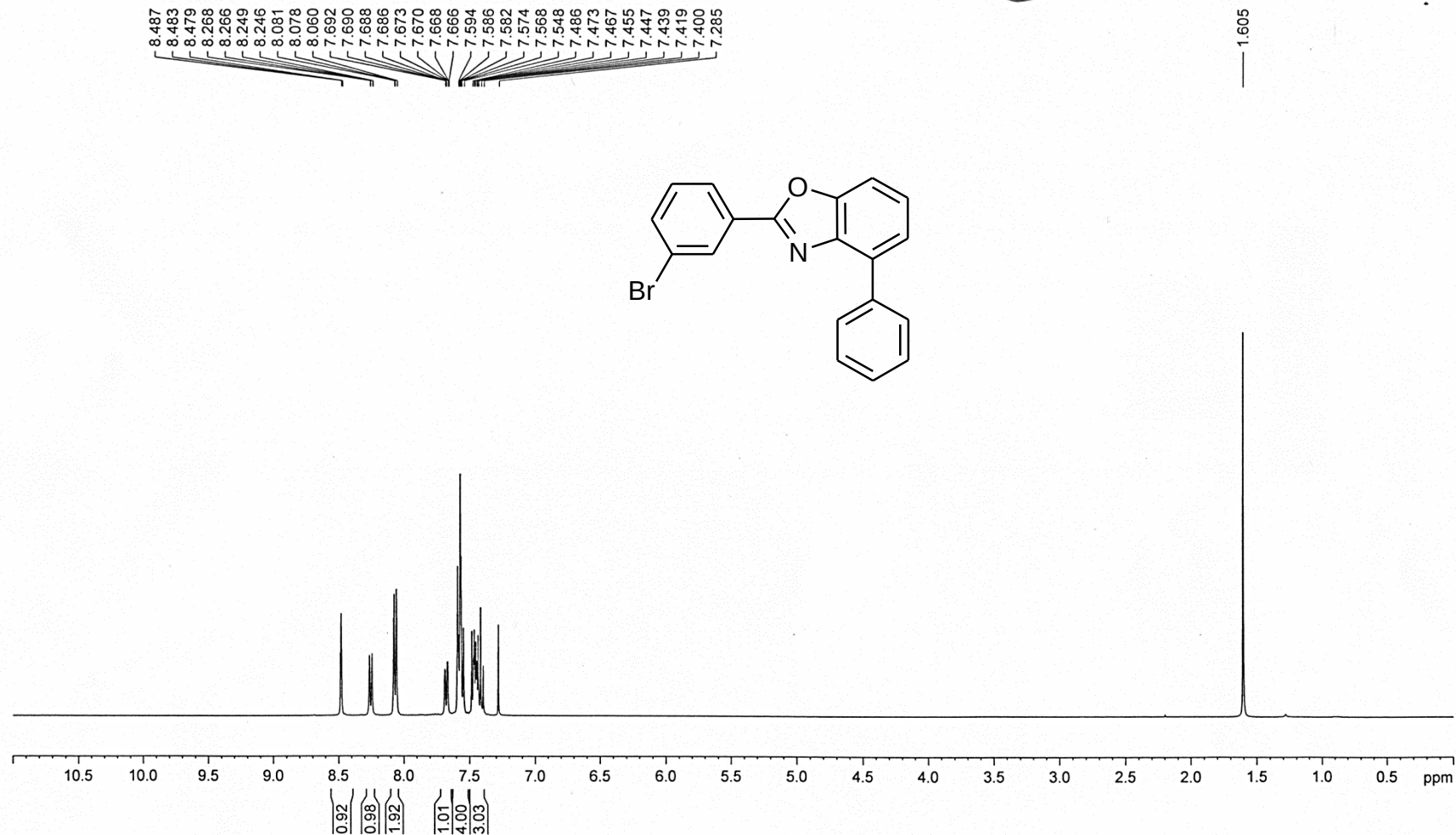
^{13}C of NP-KS-717 (Br)



^1H NMR of 2-(3-bromophenyl)-4-phenylbenzo[d]oxazole (3ja)

^1H of NP-KS-772 26.9.2019

3ja



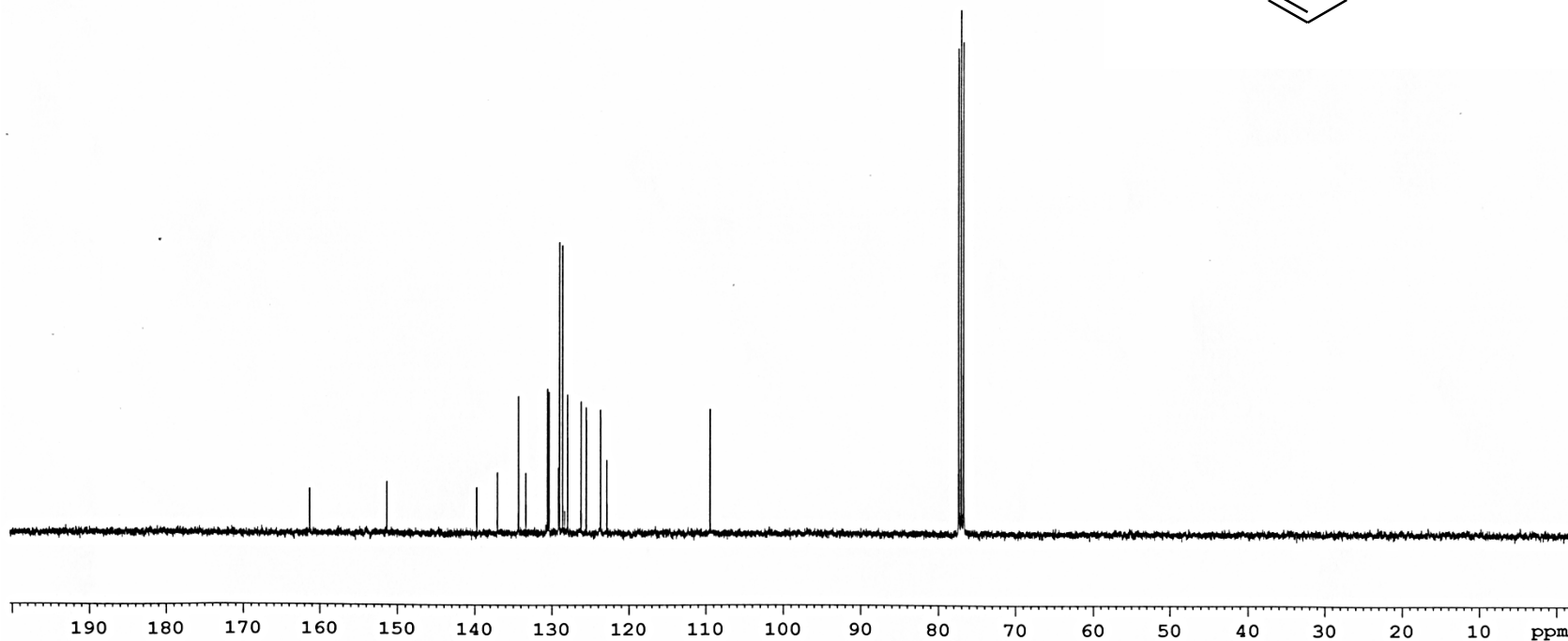
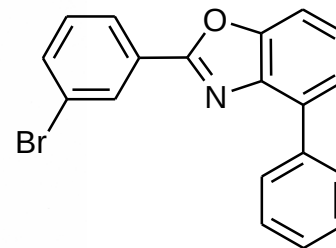
¹³C NMR of 2-(3-bromophenyl)-4-phenylbenzo[d]oxazole (3ja)

13C of NP-KS-745

7.8.2019

161.33
151.39
139.76
137.07
134.32
133.38
130.60
130.39
129.17
129.04
128.66
127.99
126.26
125.61
123.73
122.93
109.50

77.38
77.06
76.74



¹H NMR of 2-(4-nitrophenyl)-4-phenylbenzo[d]oxazole (3ka)

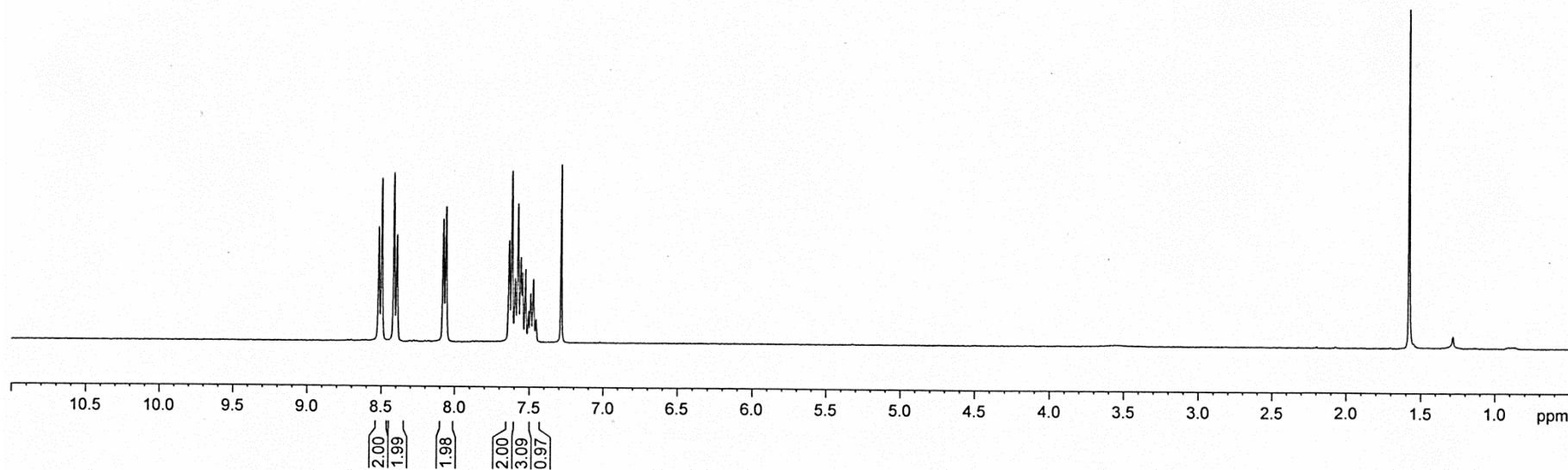
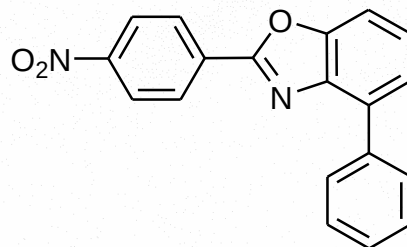
1H of NP-KS-715(NO2)

27.5.2019

3ka

8.516
8.495
8.413
8.392
8.077
8.058
7.635
7.615
7.594
7.575
7.556
7.544
7.525
7.505
7.490
7.472
7.453
7.285

1.576



¹³C NMR of 2-(4-nitrophenyl)-4-phenylbenzo[d]oxazole (3ka)

¹³C of NP-KS-71 (NO₂)

— 160.52

— 151.63

— 149.35

— 139.77

— 136.83

— 133.90

— 132.87

— 129.04

— 128.69

— 128.53

— 128.17

— 126.40

— 124.15

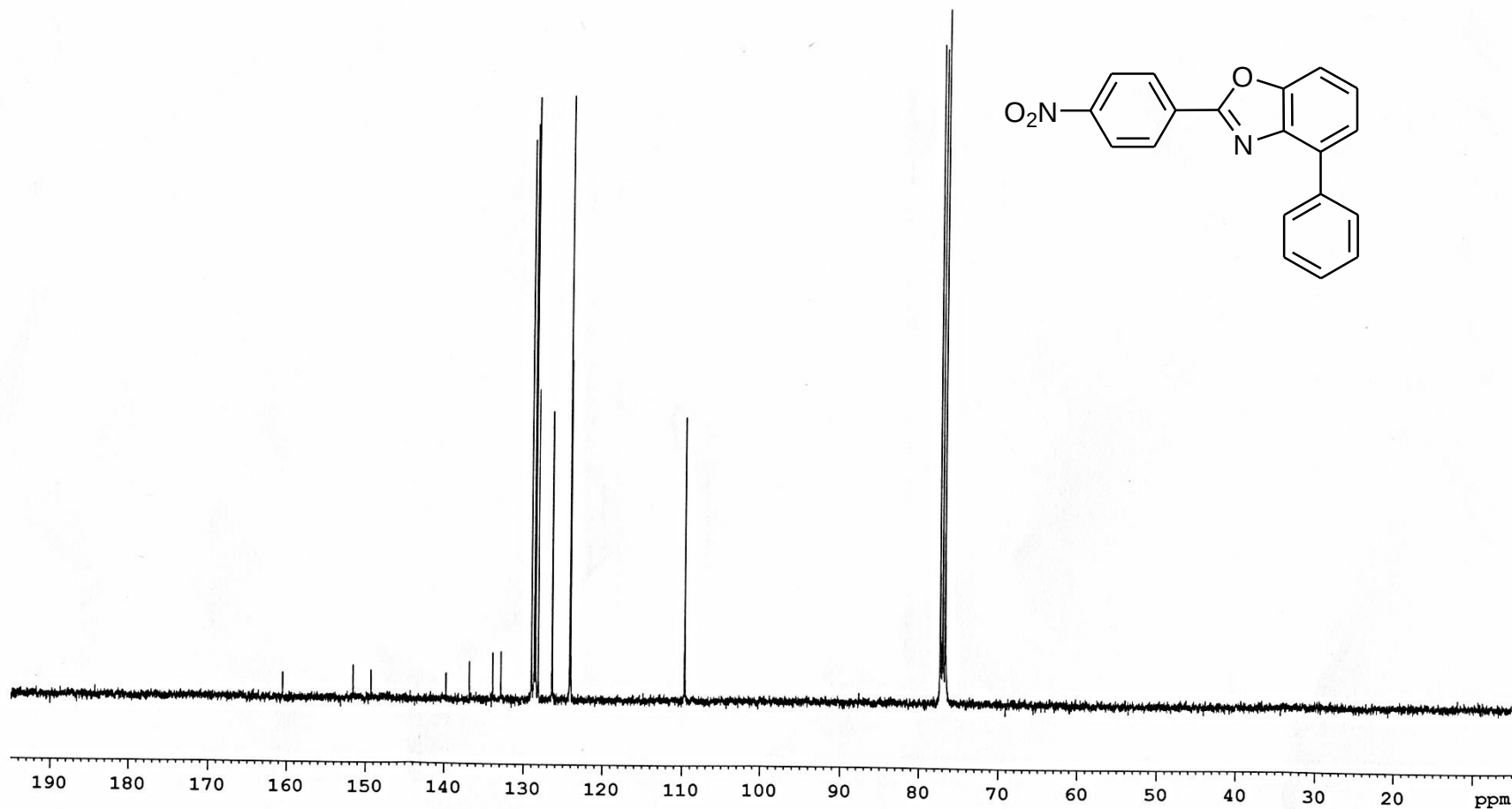
— 124.08

— 109.68

77.34

77.03

76.71

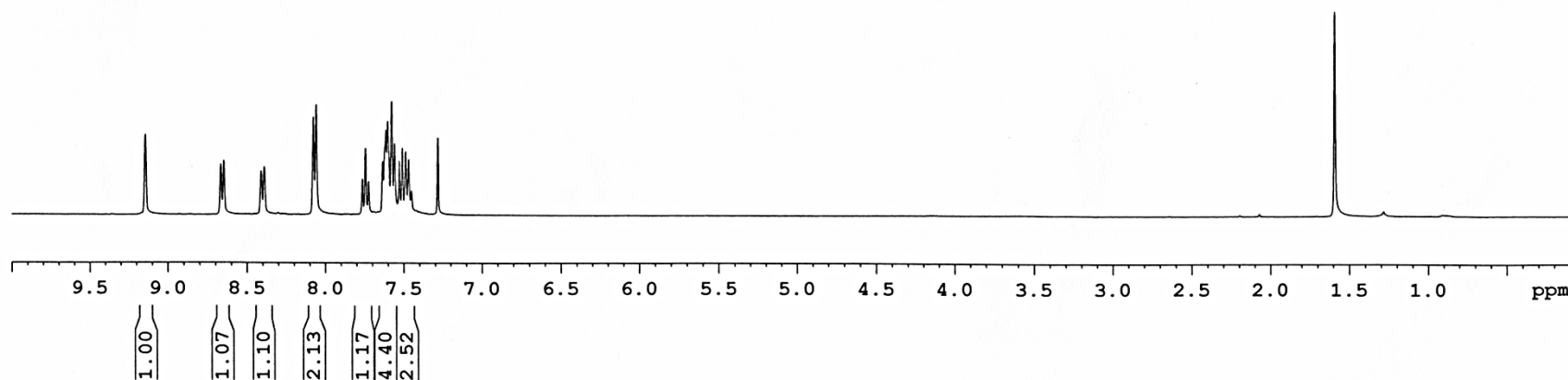
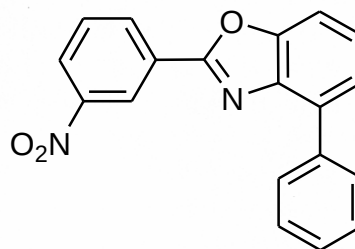


¹H NMR of 2-(3-nitrophenyl)-4-phenylbenzo[d]oxazole (3la)

¹H of NP-KS-716 28.5.2019

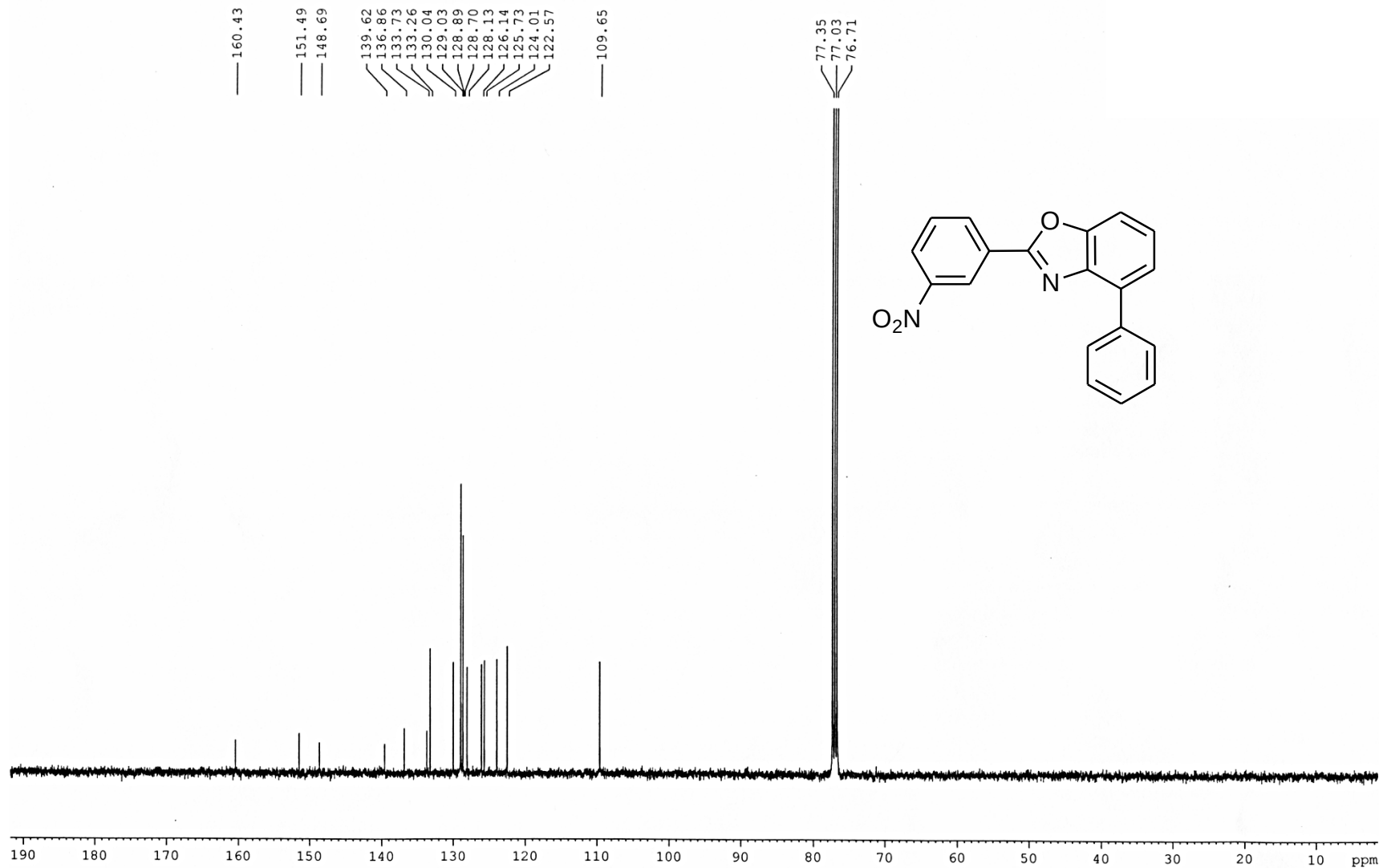
9.143
8.667
8.648
8.413
8.392
8.080
8.060
7.766
7.746
7.726
7.638
7.618
7.606
7.581
7.562
7.532
7.512
7.492
7.473
7.454
7.285

— 1.592



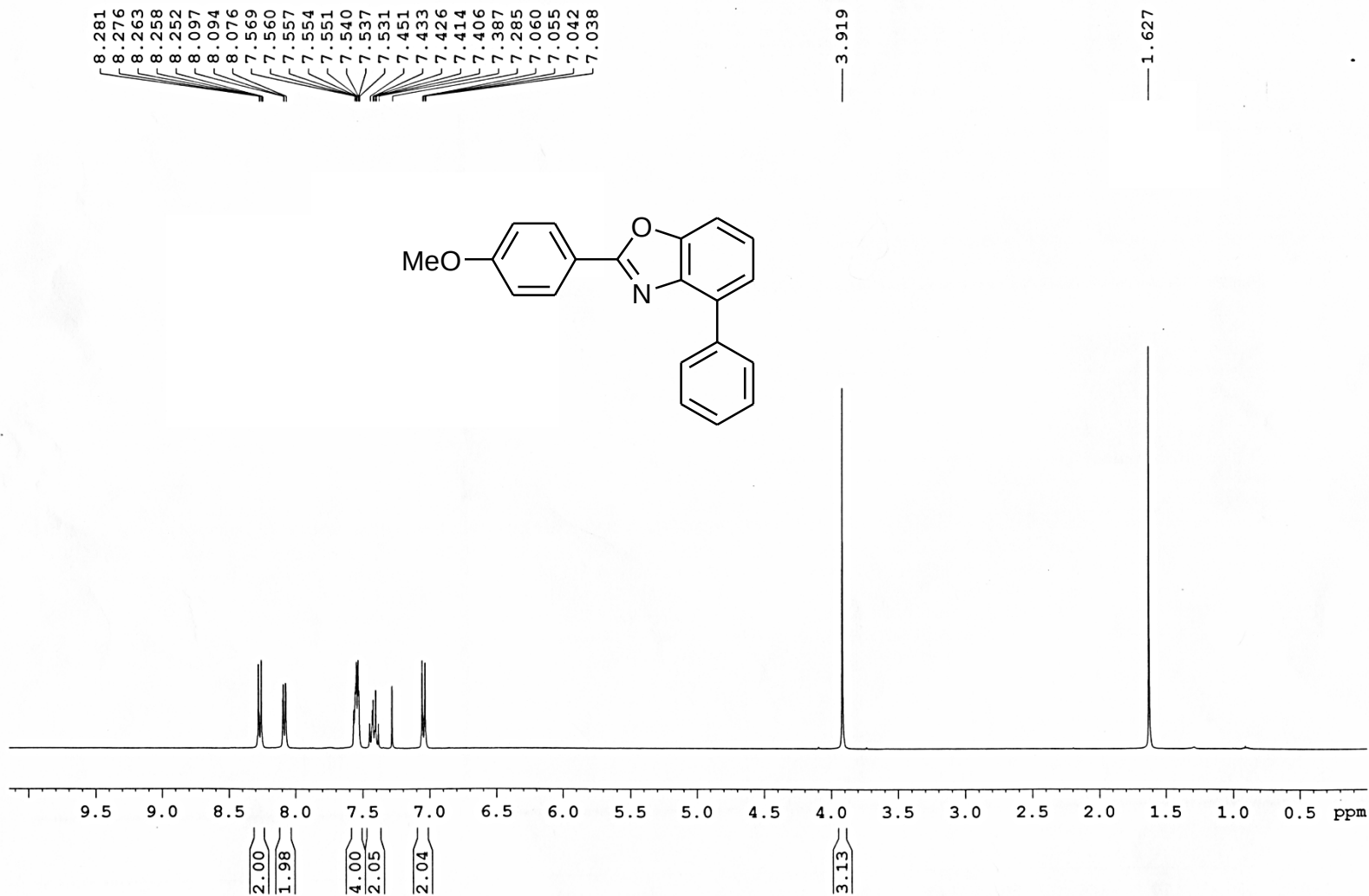
^{13}C NMR of 2-(3-nitrophenyl)-4-phenylbenzo[d]oxazole (3la)

^{13}C of NP-KS-716 29.5.2019



¹H NMR of 2-(4-methoxyphenyl)-4-phenylbenzo[d]oxazole (3ma)

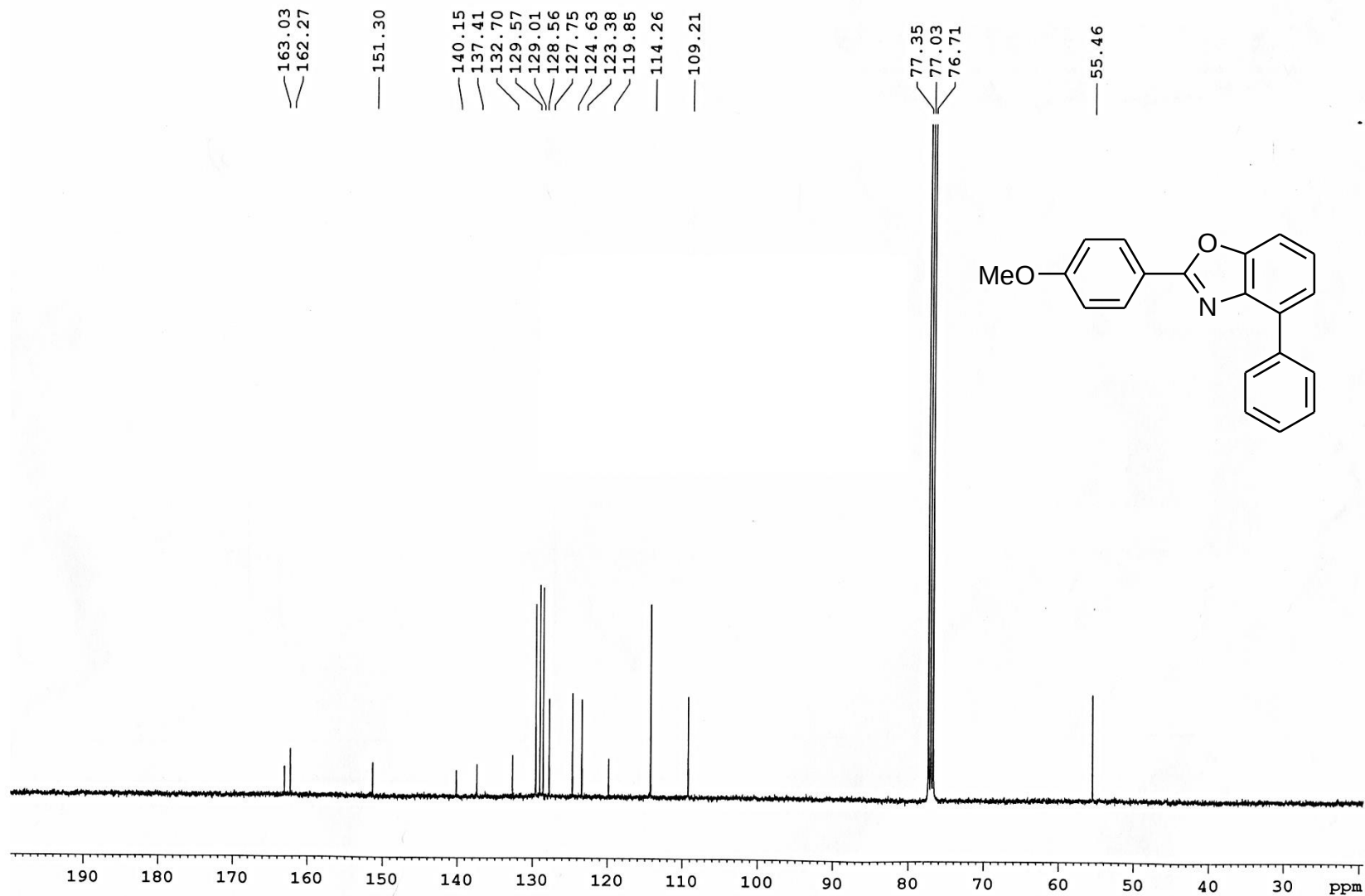
¹H of NP-KS-738 25.7.2019



¹³C NMR of 2-(4-methoxyphenyl)-4-phenylbenzo[d]oxazole (3ma)

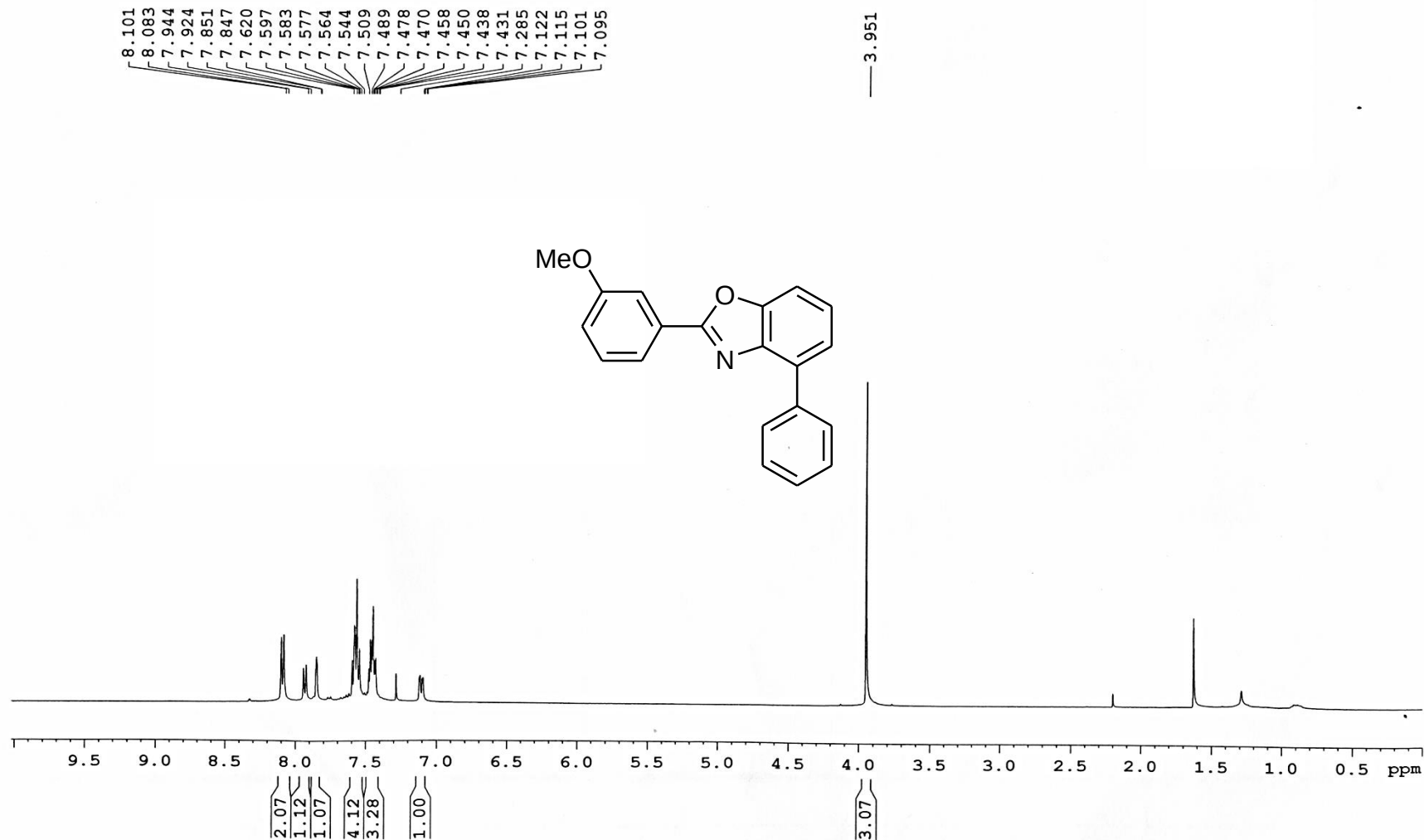
¹³C of NP-KS-738

24.7.2019



^1H NMR of 2-(3-methoxyphenyl)-4-phenylbenzo[d]oxazole (3na)

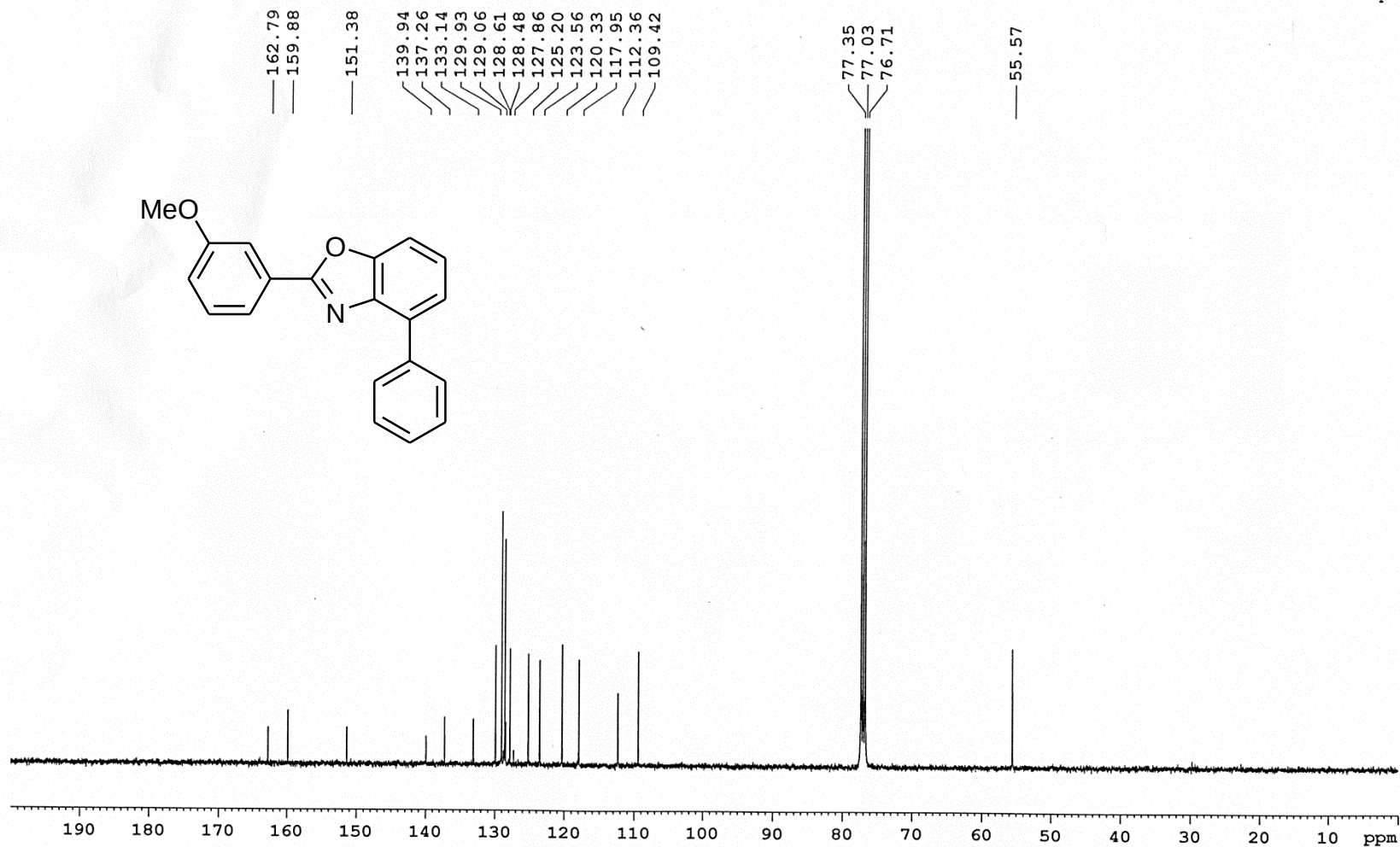
^1H of NP-KS-739(R) 31.7.2019



^{13}C NMR of 2-(3-methoxyphenyl)-4-phenylbenzo[d]oxazole (3na)

^{13}C of NP-KS-3na

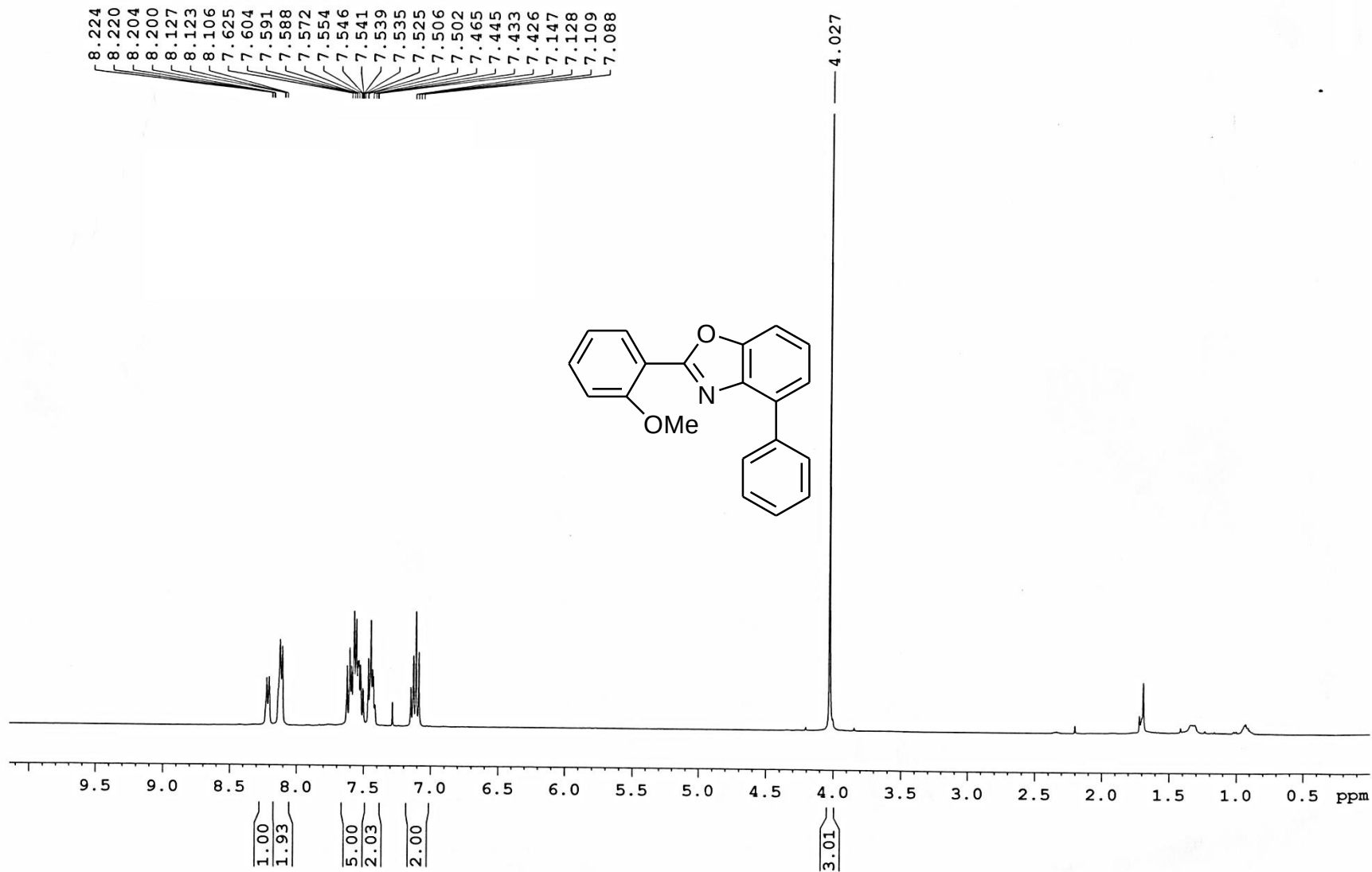
13.2.2020-



¹H NMR of 2-(2-methoxyphenyl)-4-phenylbenzo[d]oxazole (30a)

¹H of NP-KS-743

5.8.2019



^{13}C NMR of 2-(2-methoxyphenyl)-4-phenylbenzo[d]oxazole (30a)

^{13}C NMR of NP-KS-743

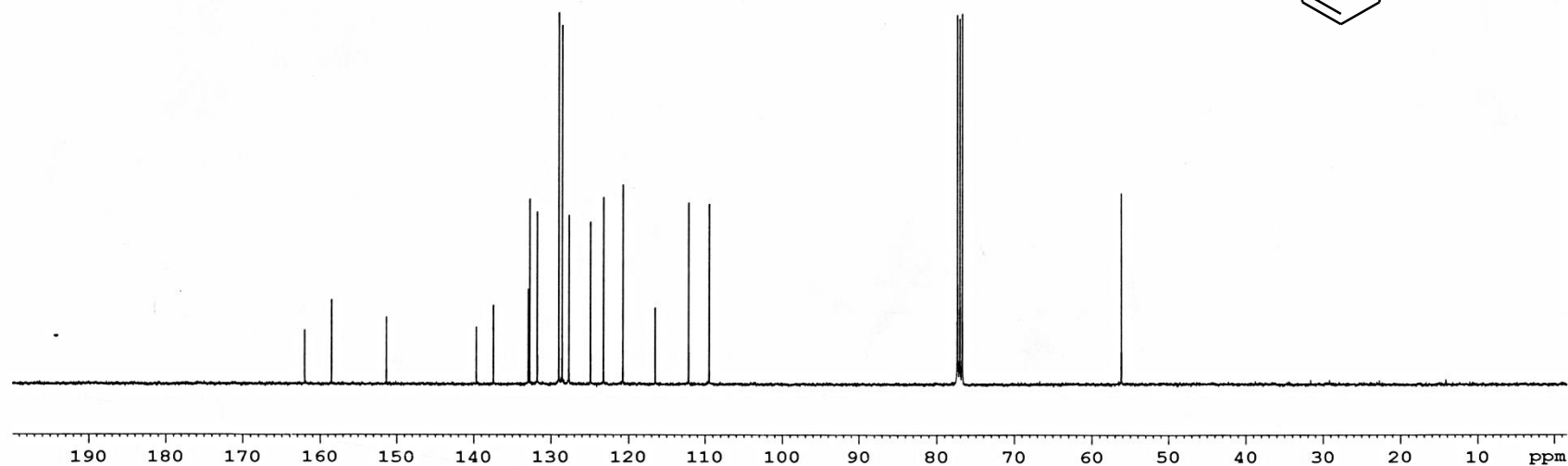
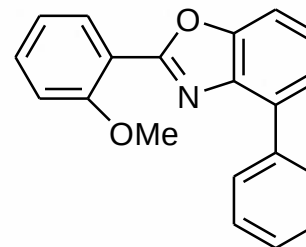
5.8.2019

— 162.03
— 158.50
— 151.33

139.71
137.47
132.94
132.74
131.77
129.03
128.58
127.72
124.94
123.28
120.77
116.54
112.16
109.50

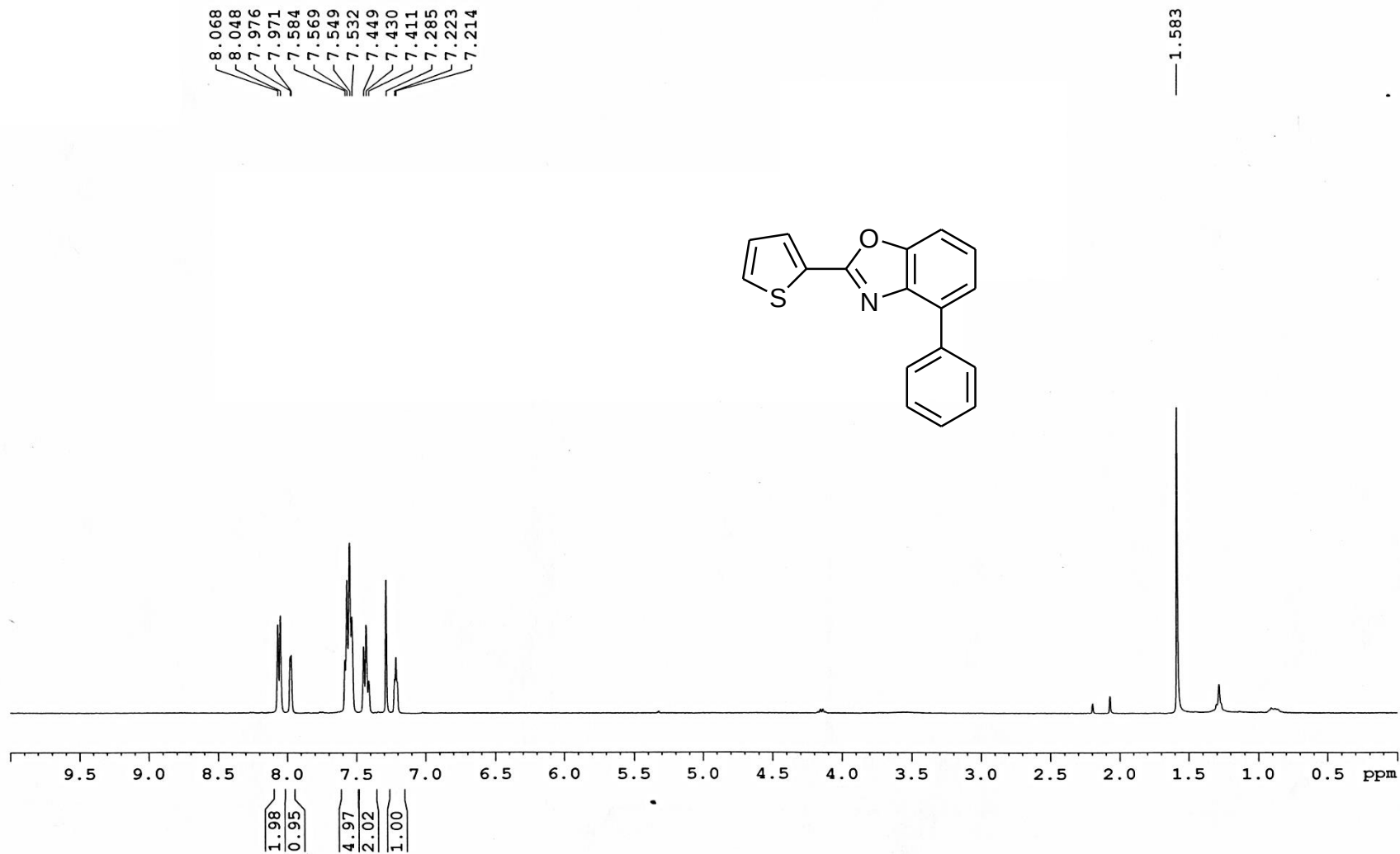
77.40
77.08
76.76

— 56.17



^1H NMR of 4-phenyl 2-(thiophen-2-yl)-benz[d]oxazole (3pa)

1h of NP-KS-713



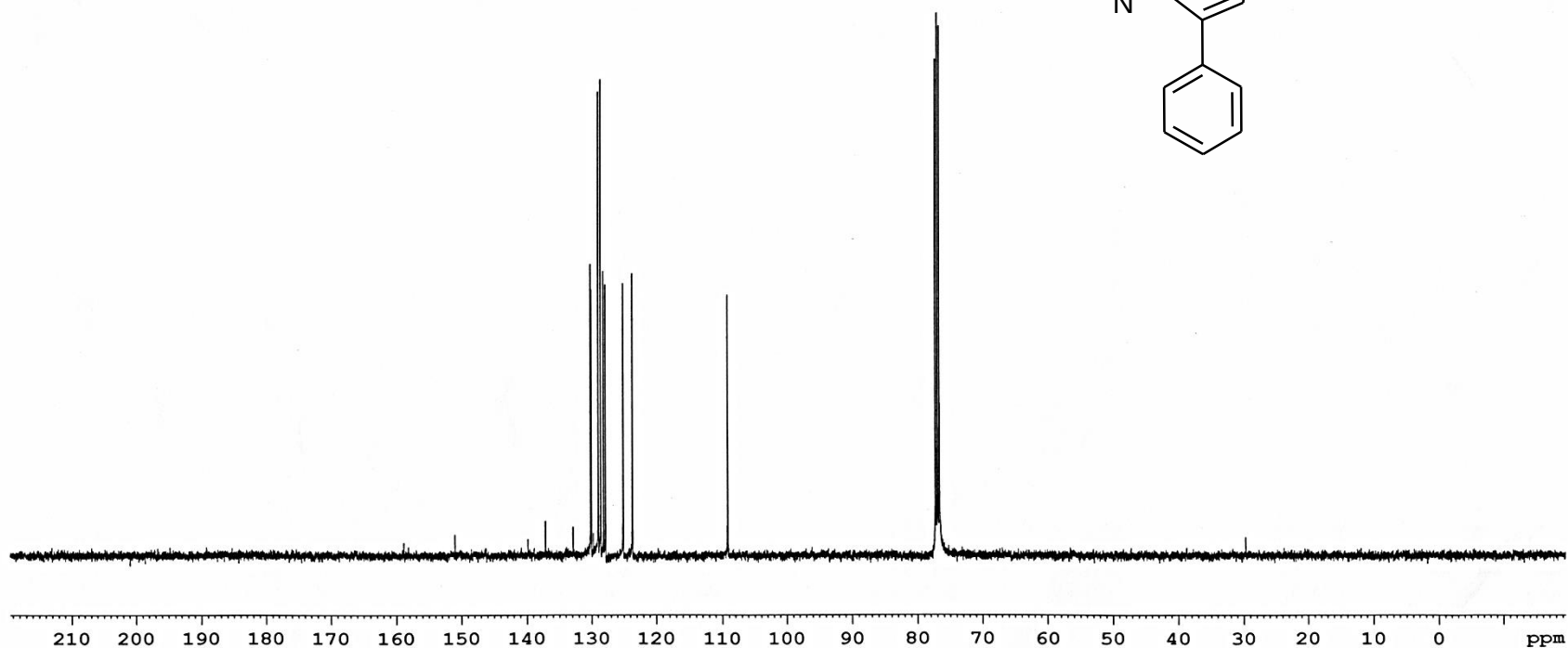
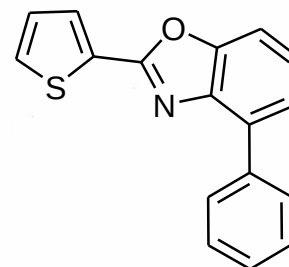
^{13}C NMR of 4-phenyl 2-(thiophen-2-yl)-benz[d]oxazole (3pa)

^{13}C of NP-KS-713

31.5.2019

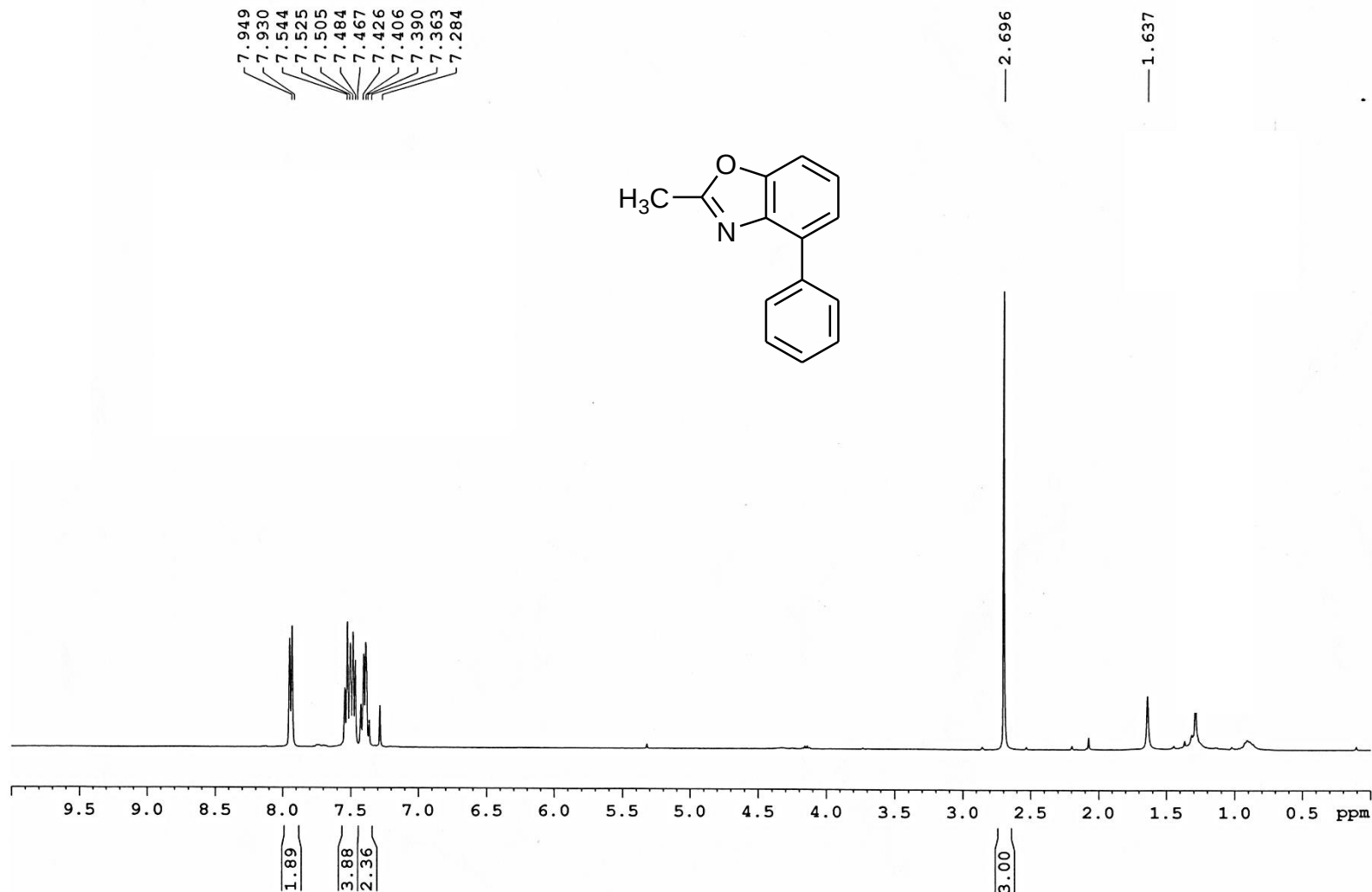
158.91
151.04
139.89
137.17
132.91
130.17
130.07
129.77
129.00
128.61
128.18
127.86
125.11
123.69
109.22

77.35
77.03
76.71

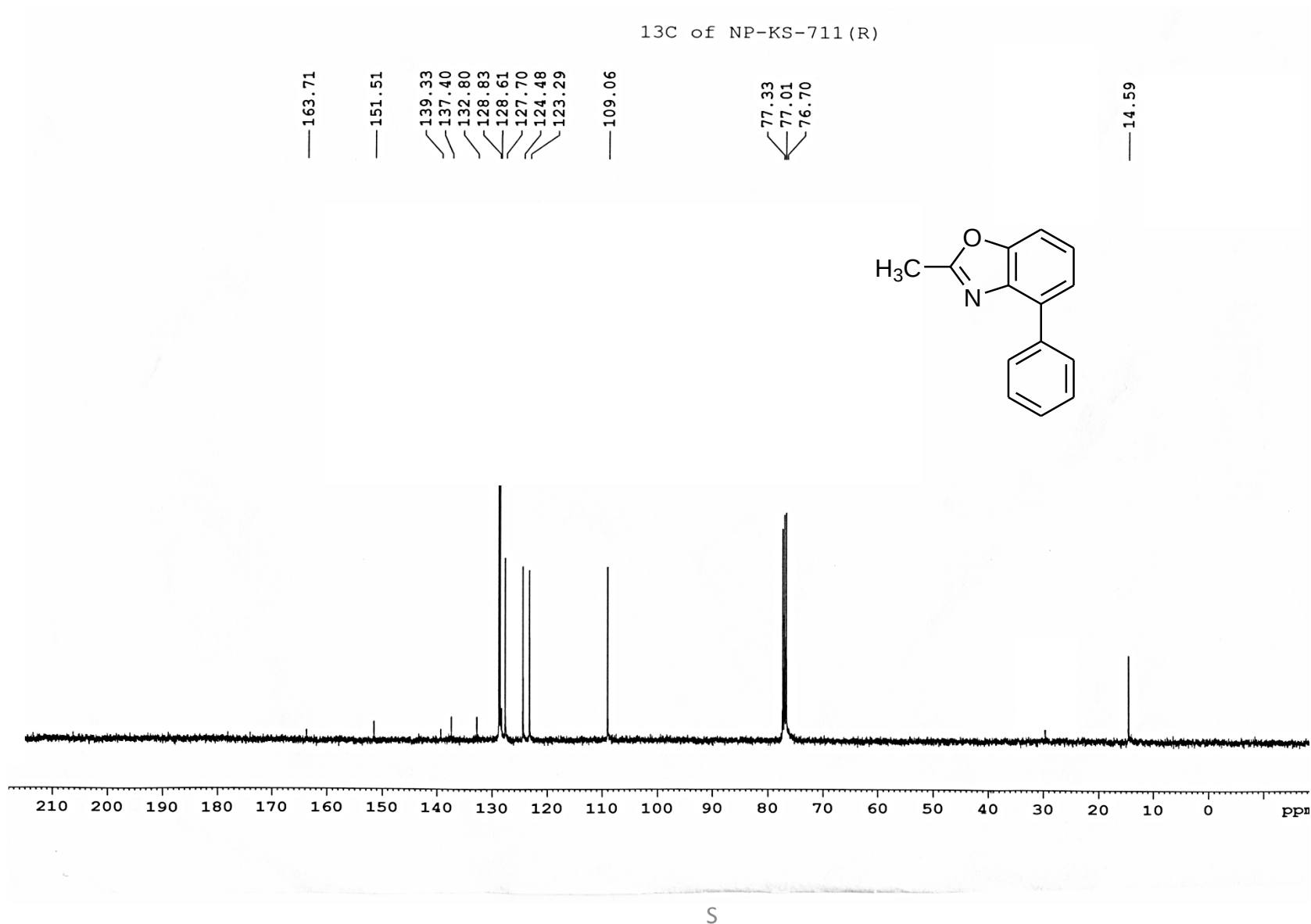


¹H NMR of 2-methyl-4-phenylbenzo[d]oxazole (3qa)

¹H of NP-KS-711 (R)

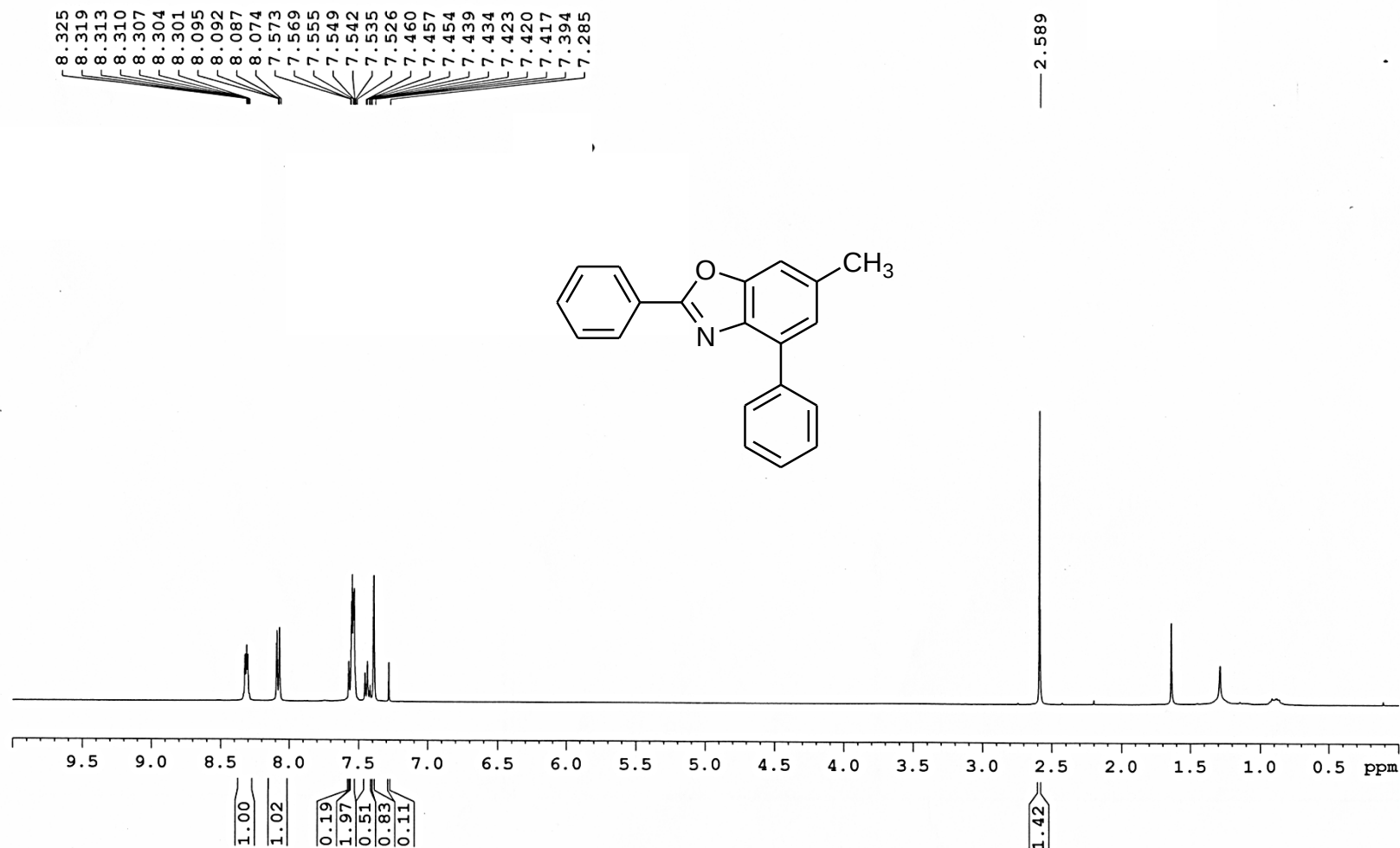


^{13}C NMR of 2-methyl-4-phenylbenzo[d]oxazole (3qa)



¹H NMR of 6-methyl-2,4-diphenylbenzo[d]oxazole (3ra)

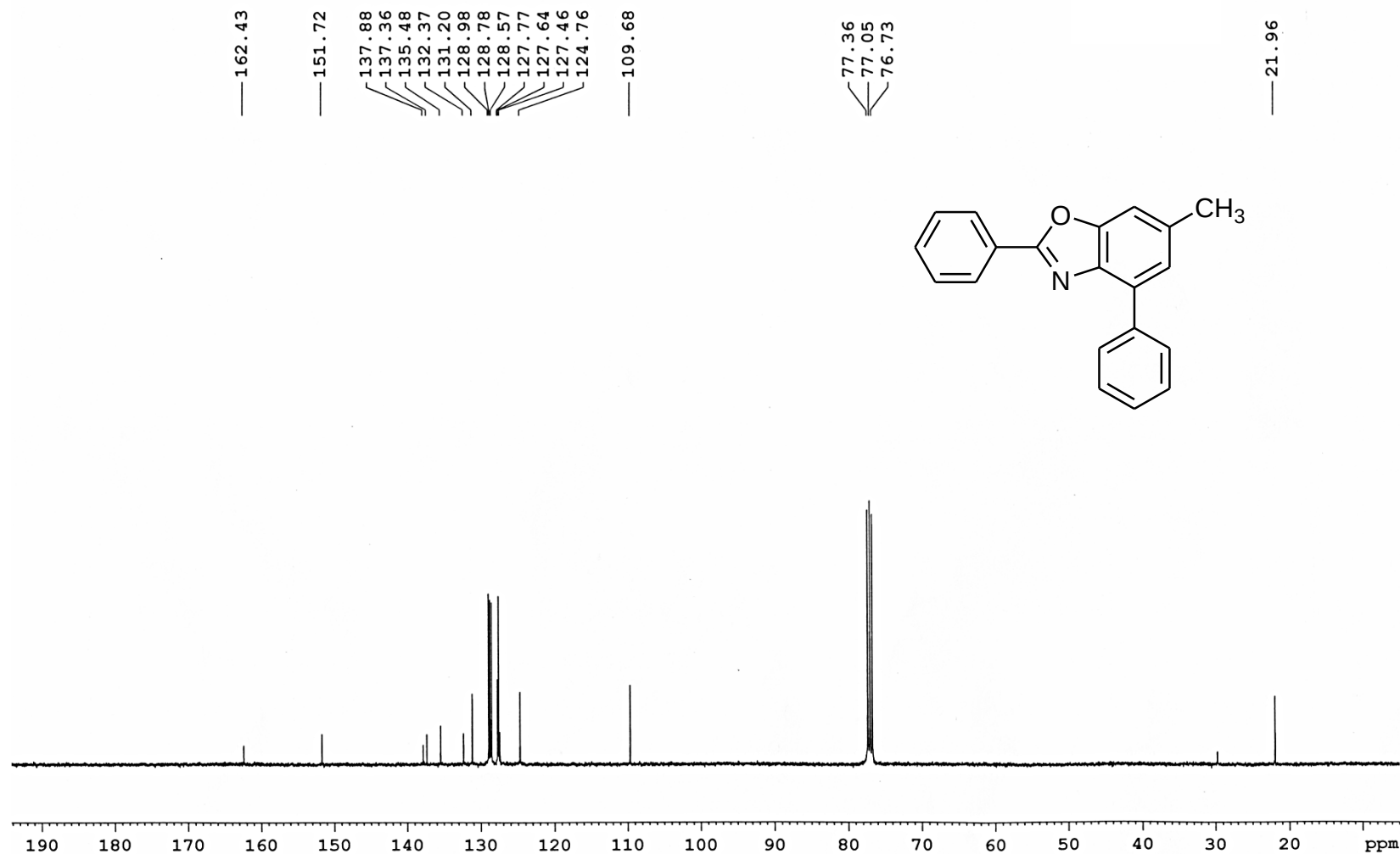
¹H of NP-KS-722 (-NH-CH3) 13.6.2019



¹³C NMR of 6-methyl-2,4-diphenylbenzo[d]oxazole (3ra)

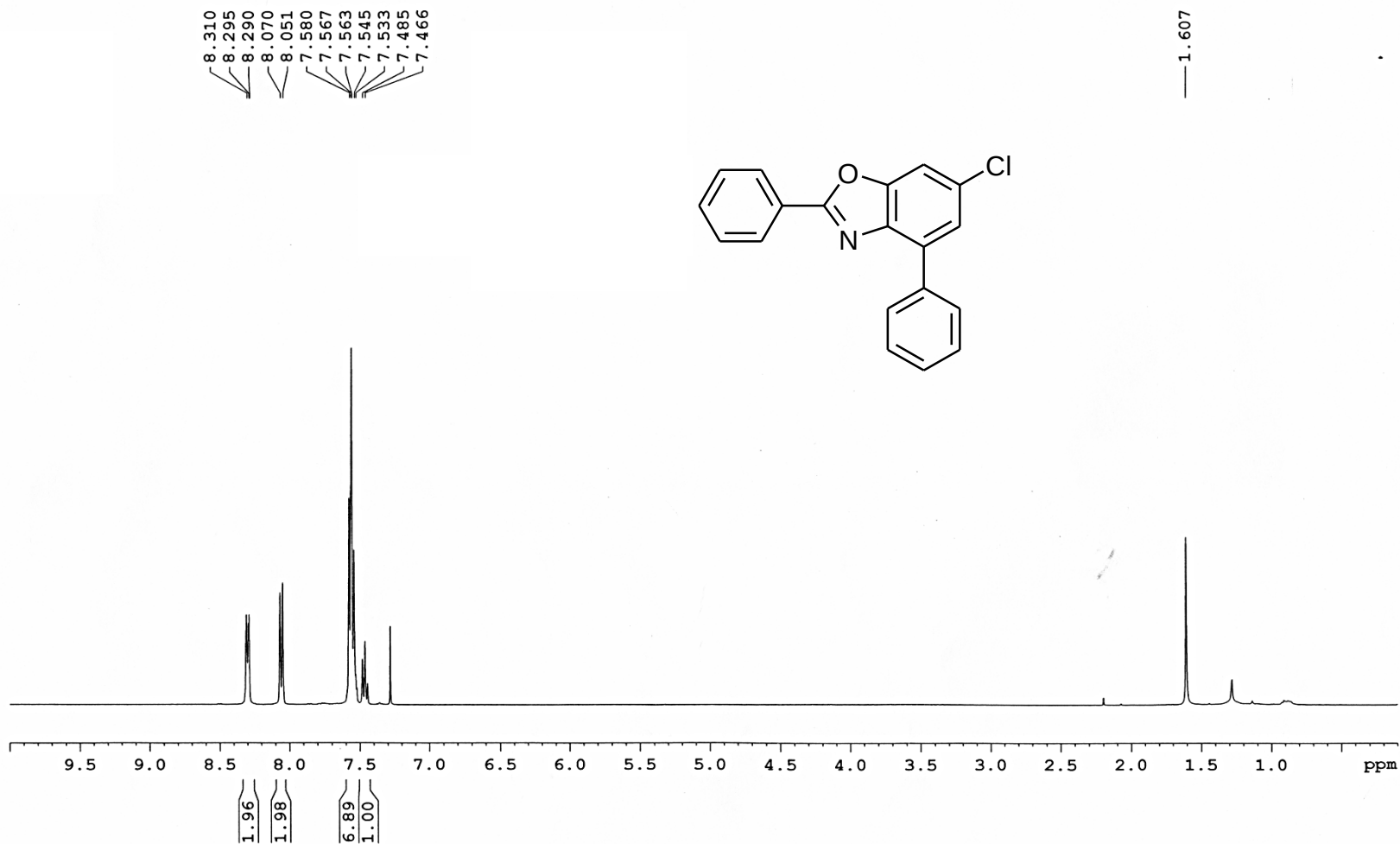
¹³C of NP_KS-722 (NH₂-CH₃)

13.6.2019



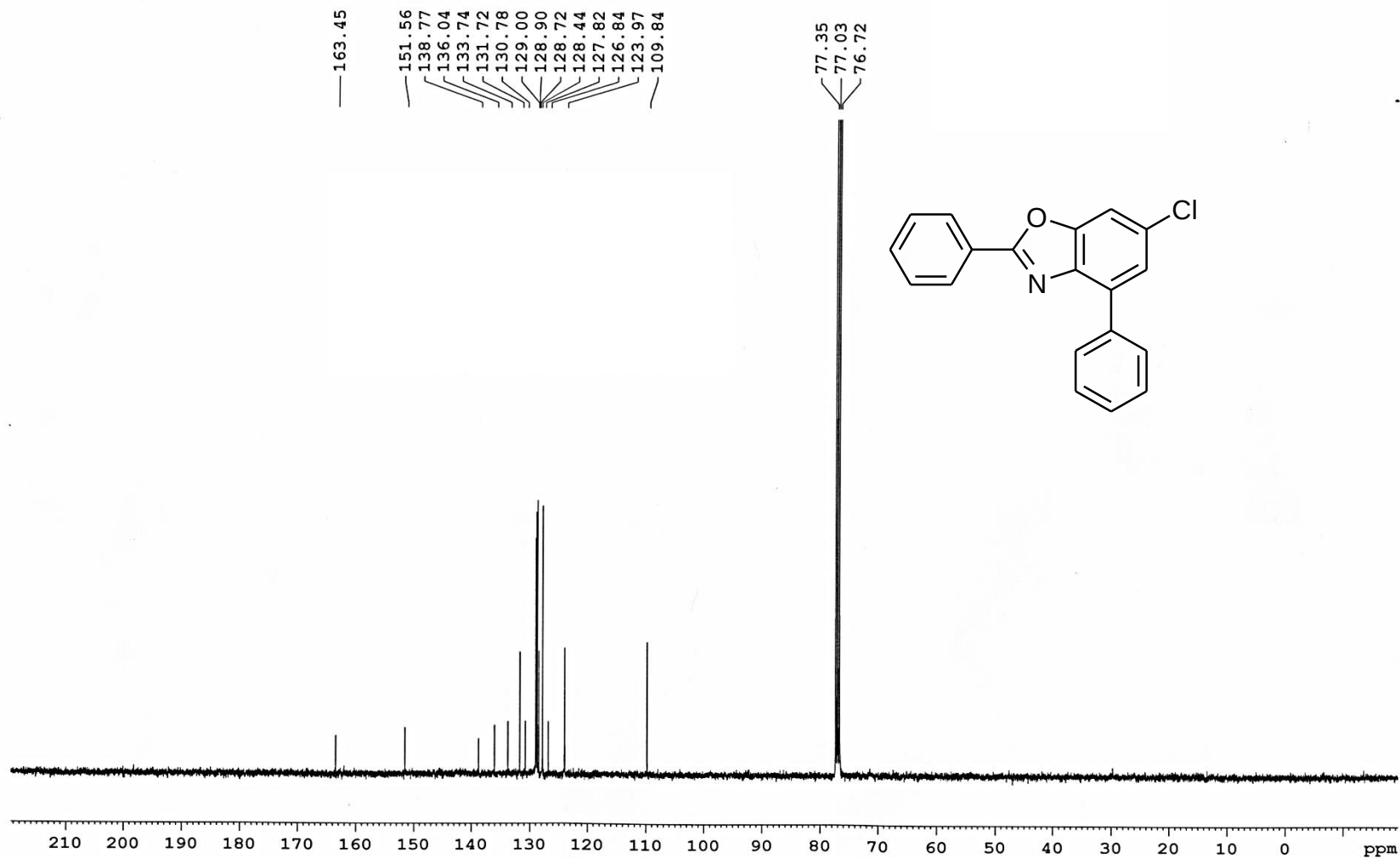
¹H NMR of 6-chloro-2,4-diphenylbenzo[d]oxazole (3sa)

¹H of NP-KS-723 (NH-Cl) 13.6.2019



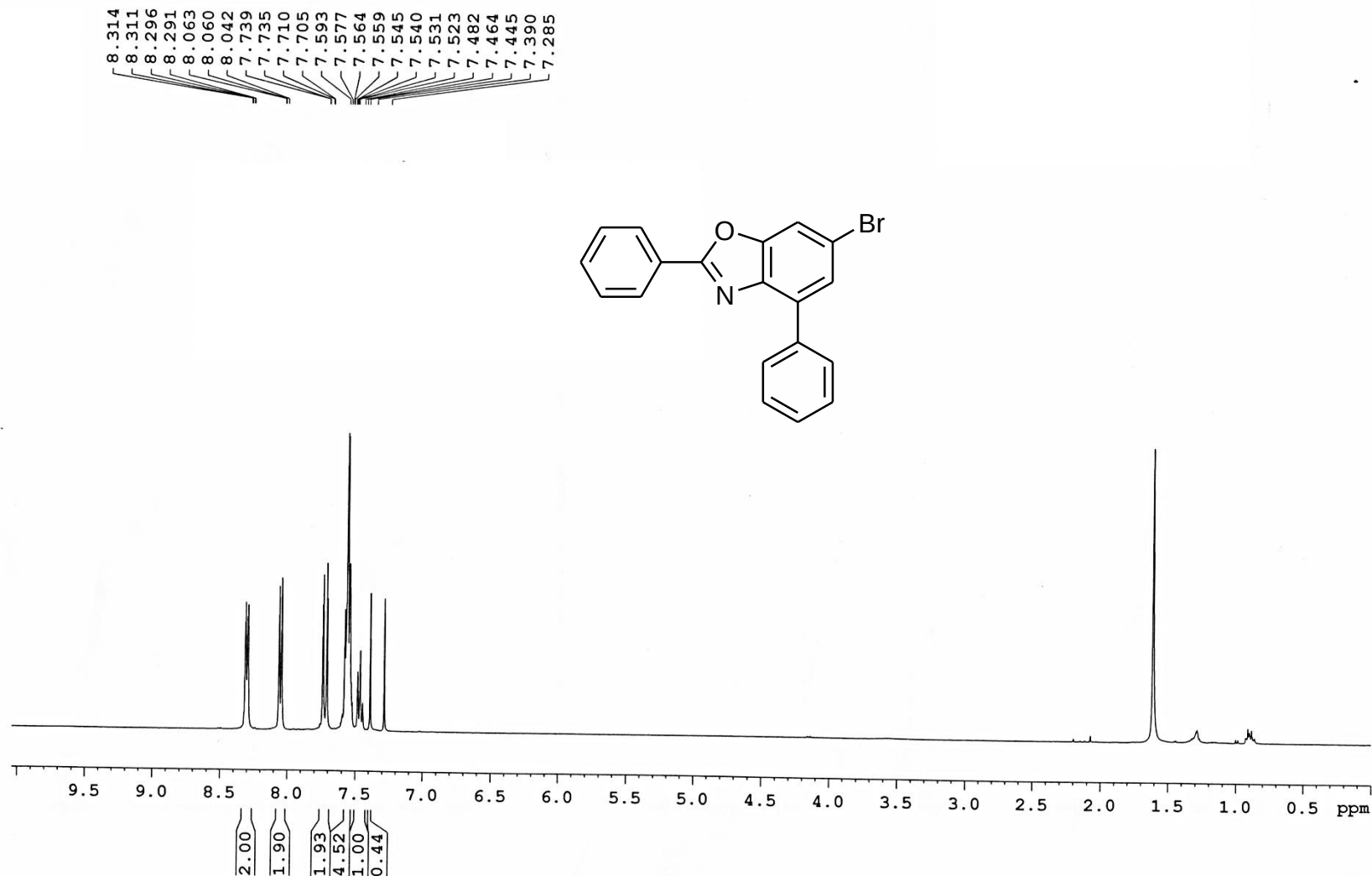
¹³C NMR of 6-chloro-2,4-diphenylbenzo[d]oxazole (3sa)

¹³C of DS-KS-723 (NH-Cl) 14.6.2019



¹H NMR of 6-bromo-2,4-diphenylbenzo[d]oxazole (3ta)

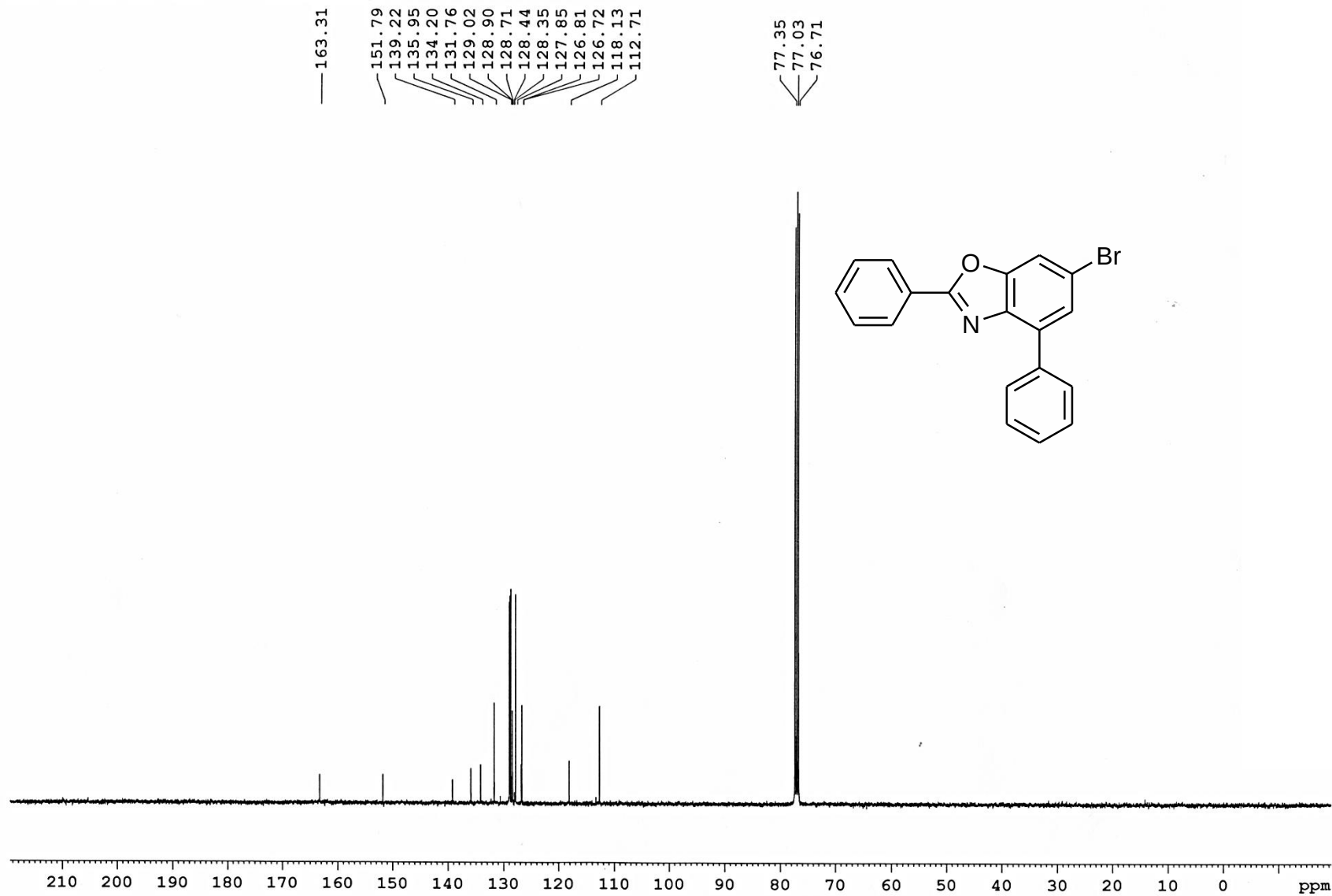
¹H of NP-KS-740 24.7.2019



^{13}C NMR of 6-bromo-2,4-diphenylbenzo[d]oxazole (3ta)

13C of NP-KS-740

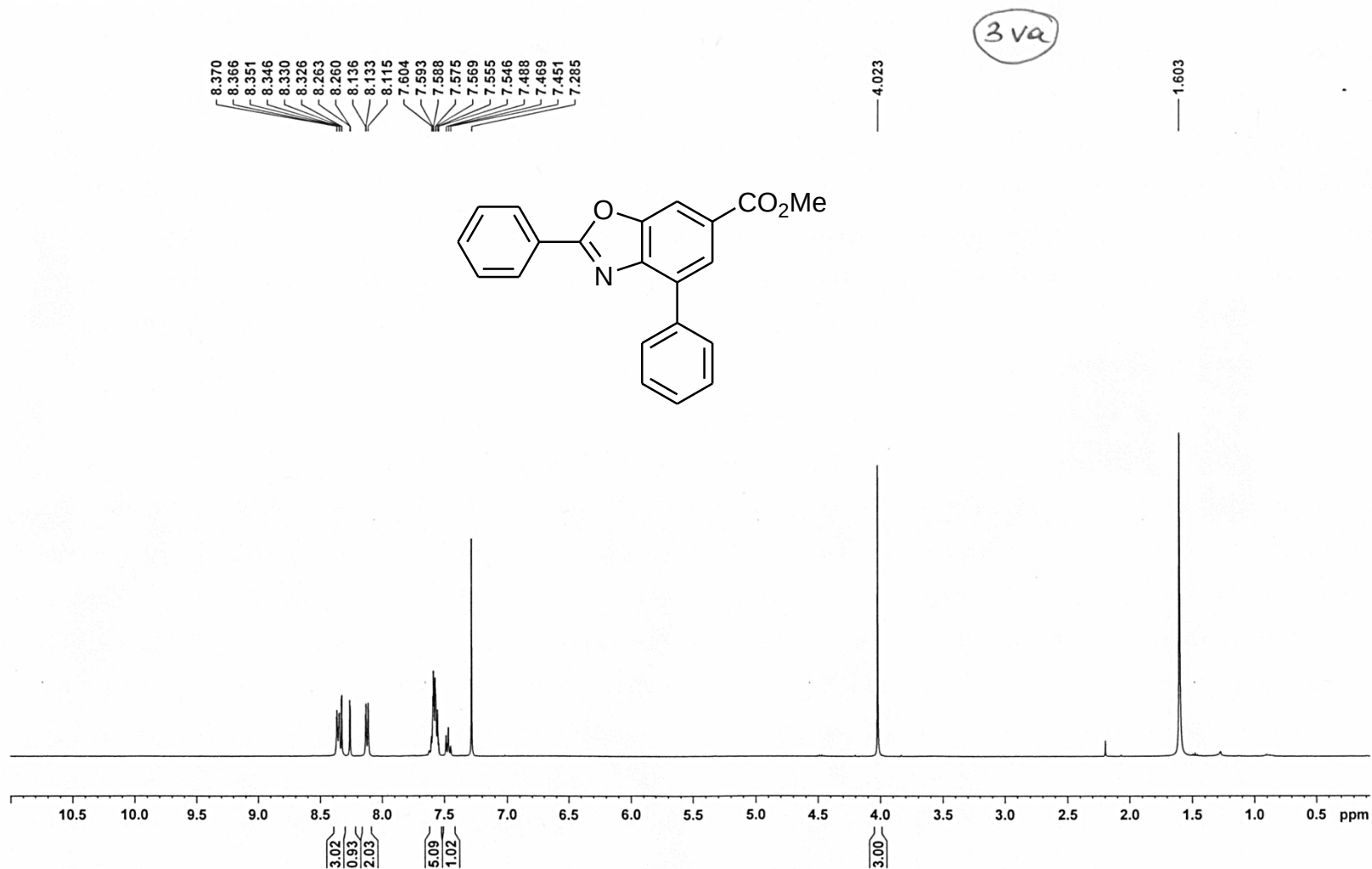
24.7.2019



¹H NMR of Methyl-2,4-diphenylbenzo[d]oxazole-6-carboxylate(3va)

¹H of NP-KS-724

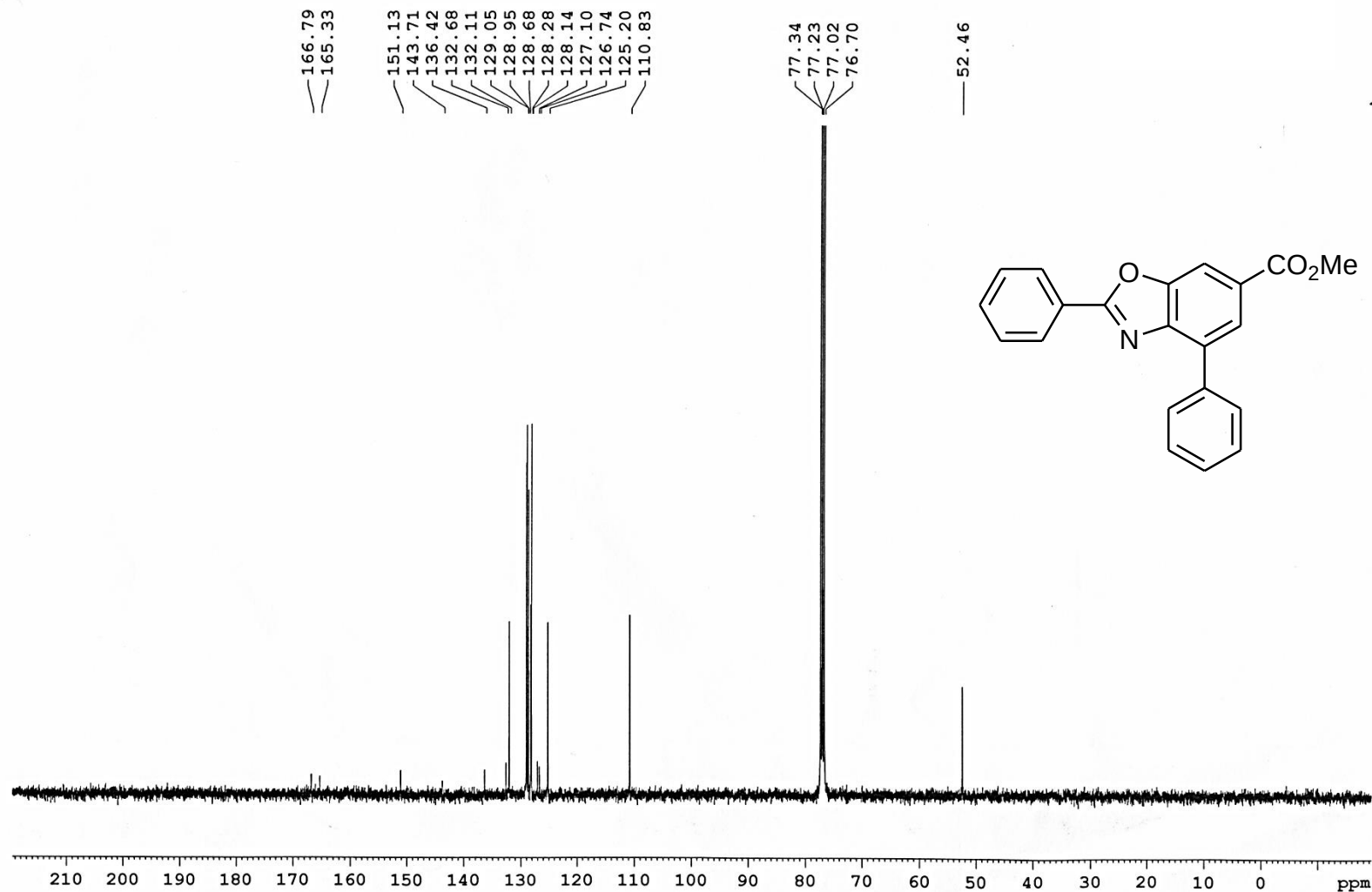
18.6.2019



¹³C NMR of Methyl-2,4-diphenylbenzo[d]oxazole-6-carboxylate(3va)

¹³C of NP-KS-724

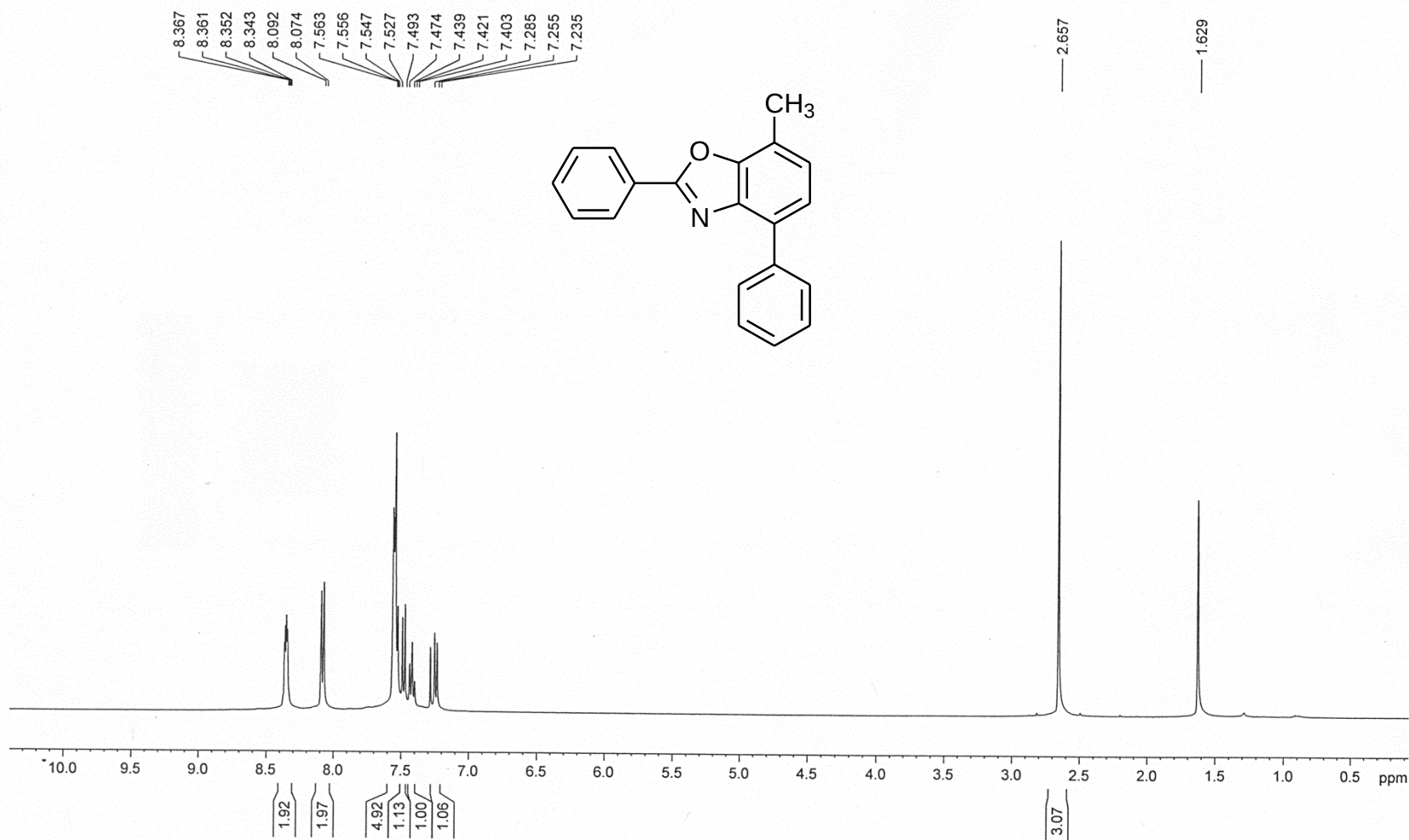
18.6.2019



¹H NMR of 7-methyl-2,4-diphenylbenzo[d]oxazole(3wa)

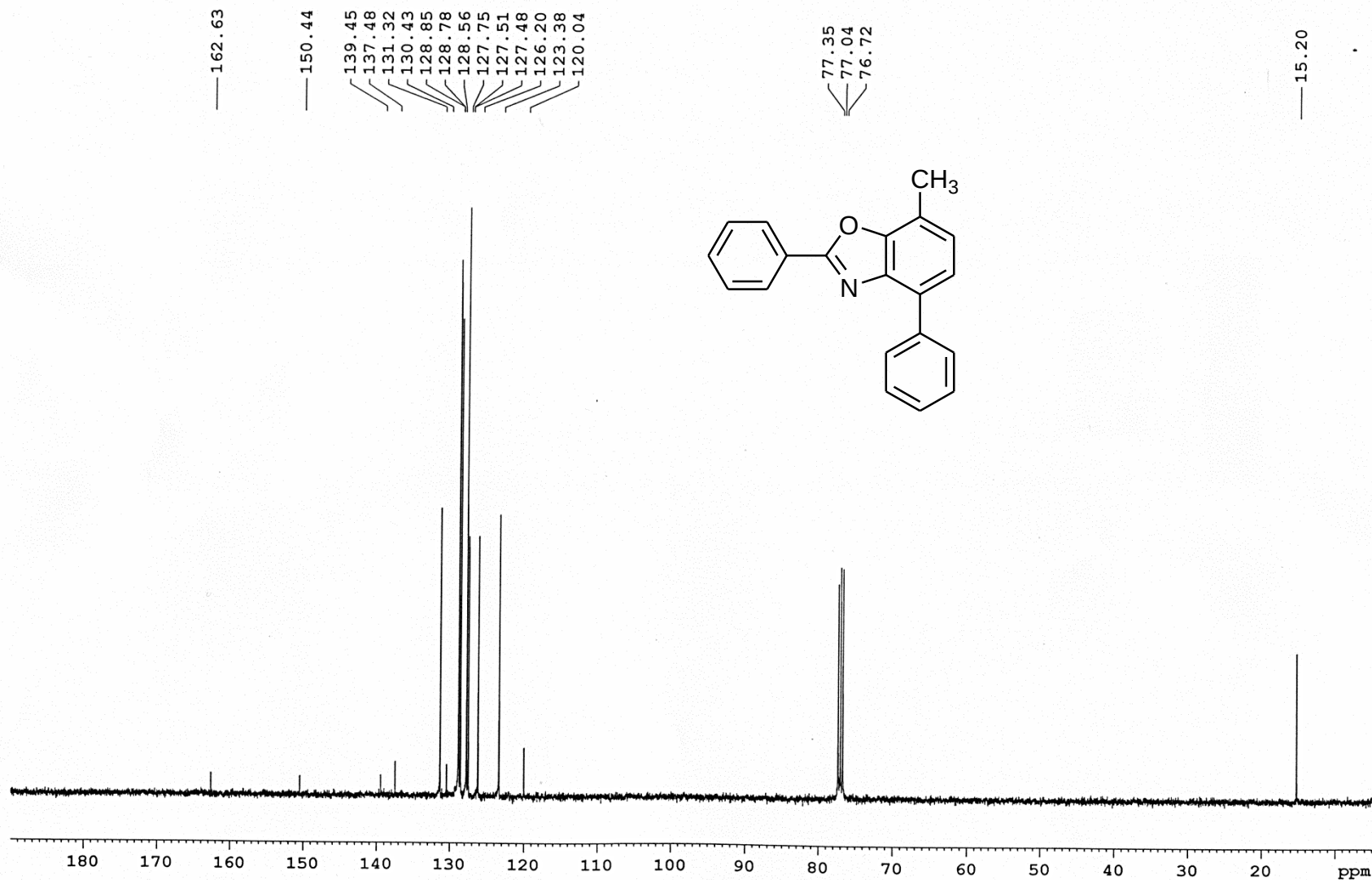
¹H of NP-KS-725 20.6.2019

3wa



^{13}C NMR of 7-methyl-2,4-diphenylbenzo[d]oxazole(3wa)

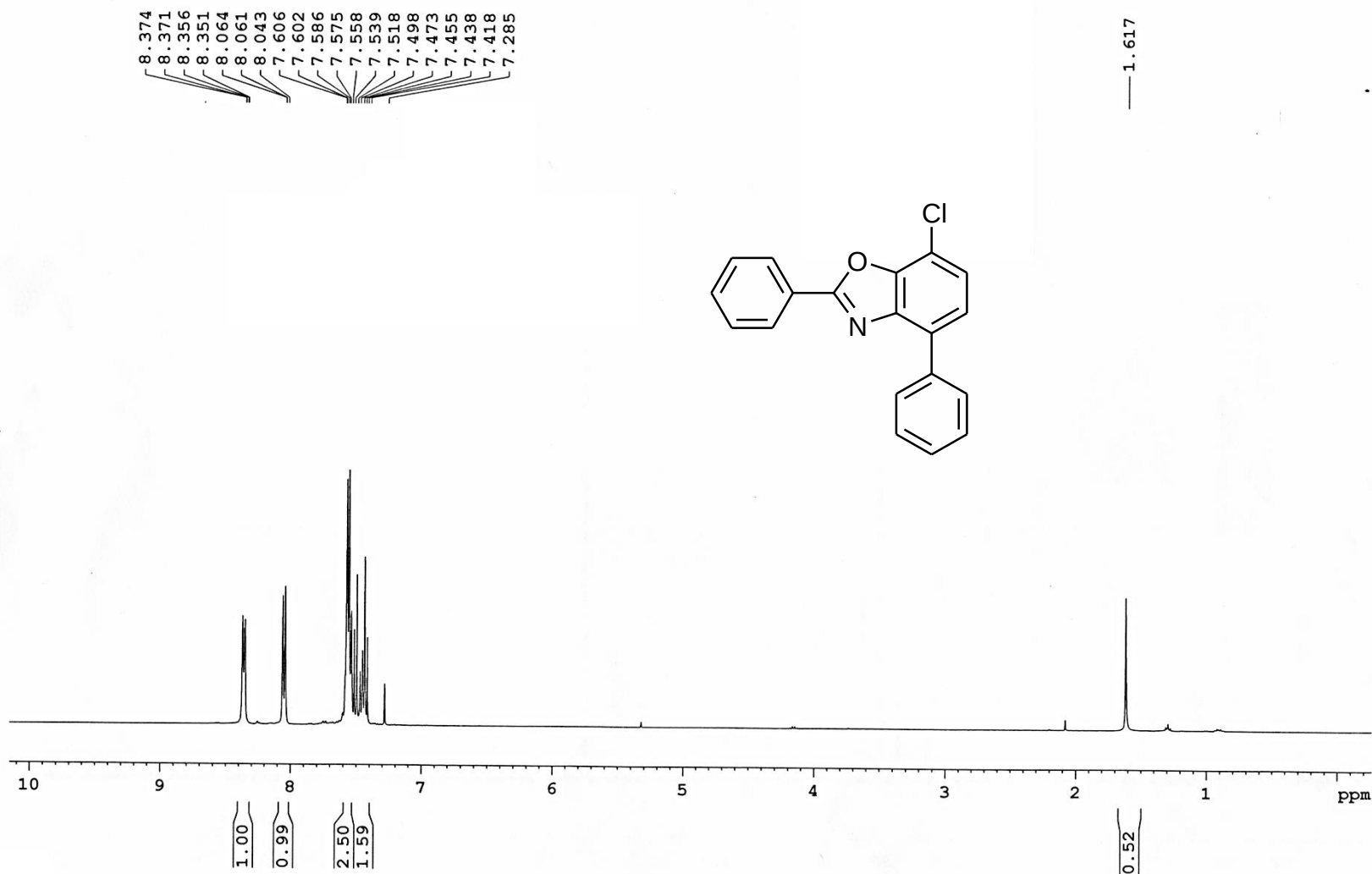
^{13}C of NP-KS-725 20.6.2019



¹H NMR of 7-chloro-2,4-diphenylbenzo[d]oxazole (3xa)

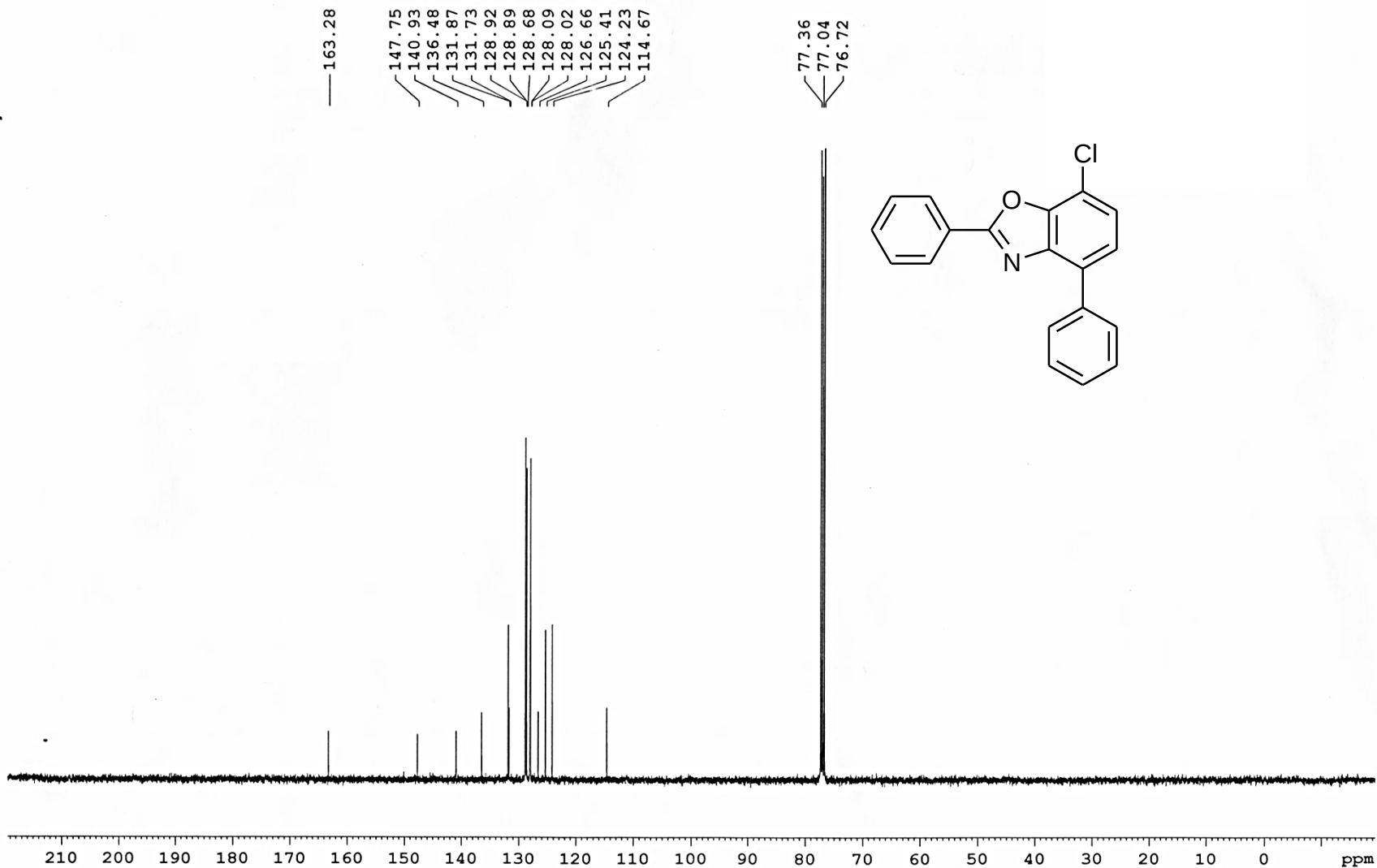
¹H of NP-KS-768

16.9.2019



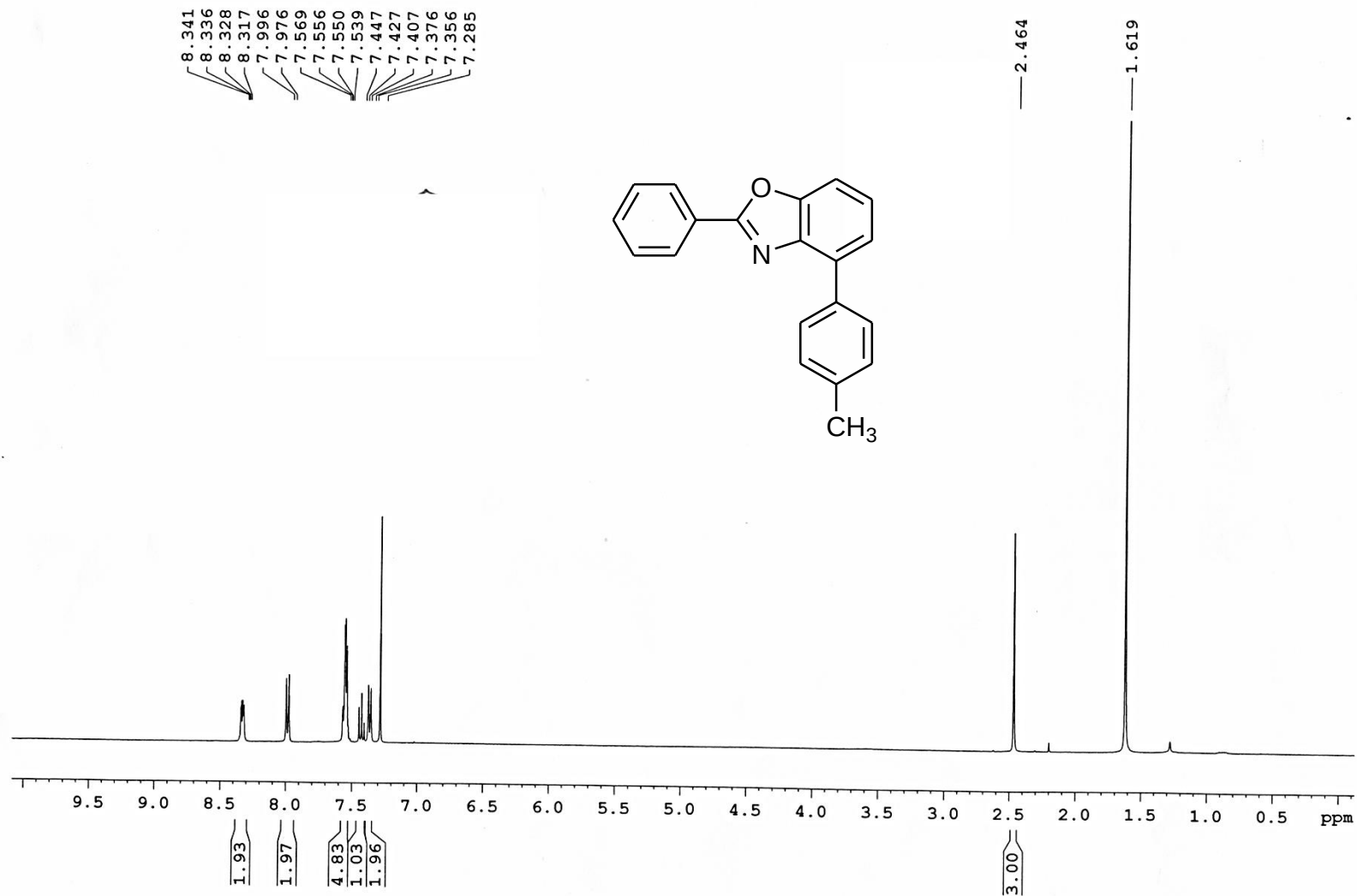
¹³C NMR of 7-chloro-2,4-diphenylbenzo[d]oxazole (3xa)

¹³C of NP-KS-768 16.9.2019



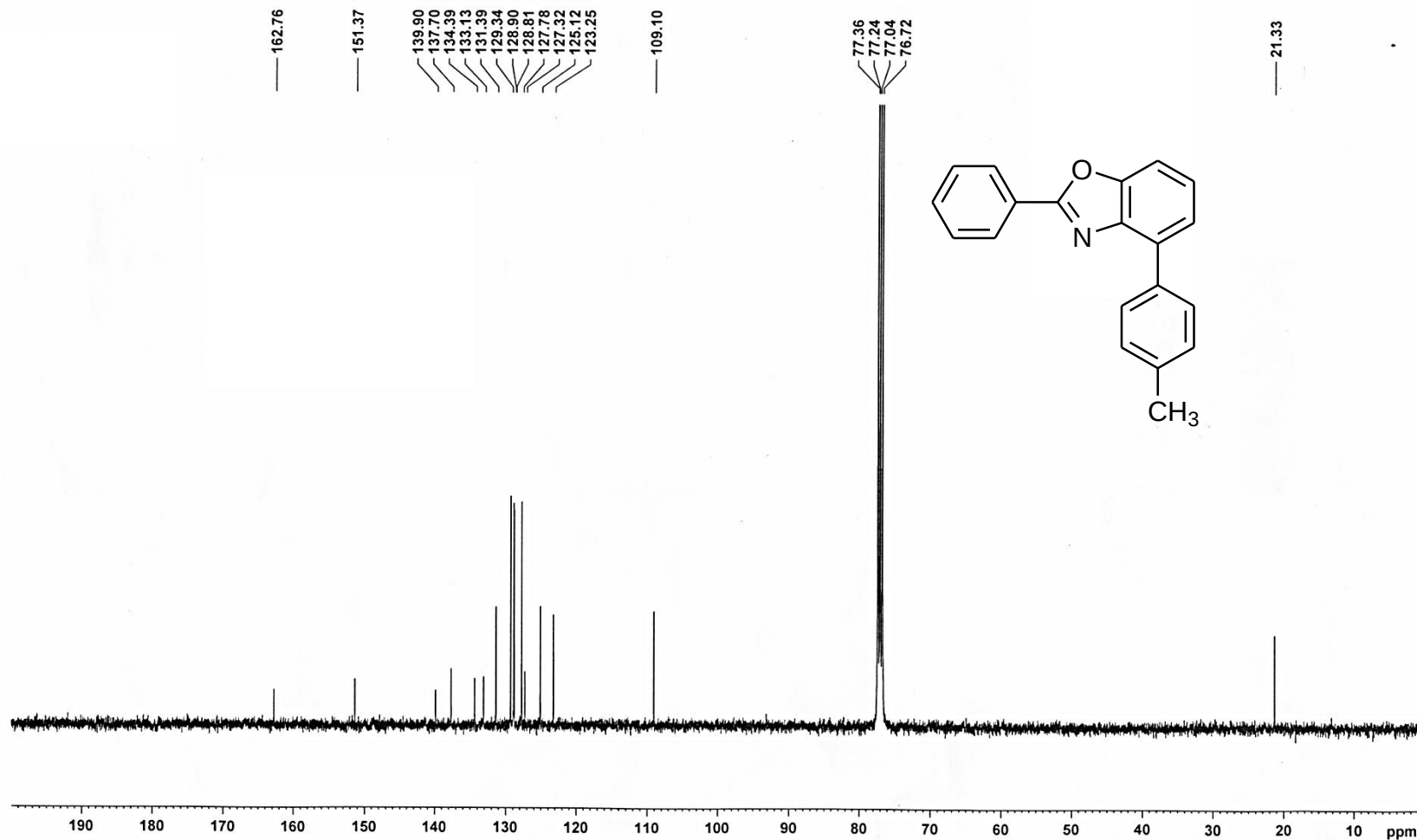
¹H NMR of 2-phenyl -4- p-tolylbenz[d]oxazole (3ab)

1H NP-KS-726 28.6.2019



¹³C NMR of 2-phenyl -4- p-tolylbenz[d]oxazole (3ab)

13C of NP-KS-726 30.6.2019



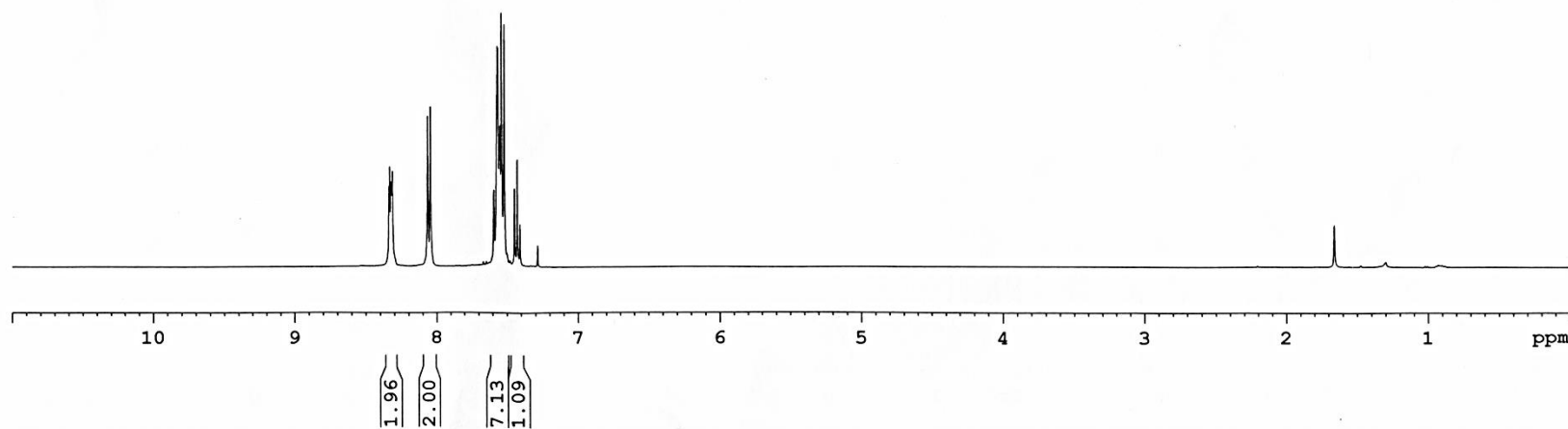
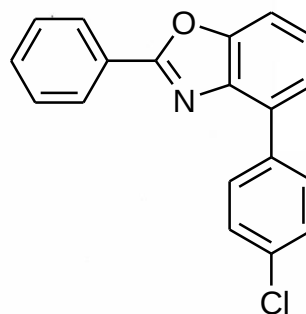
¹H NMR of 4-(4-chlorophenyl)-2-phenylbenzo[d]oxazole (3ac)

¹H of Np-KS-727

2.7.2019

8.339
8.334
8.326
8.322
8.315
8.066
8.044
7.592
7.568
7.564
7.555
7.550
7.541
7.520
7.448
7.428
7.409
7.285

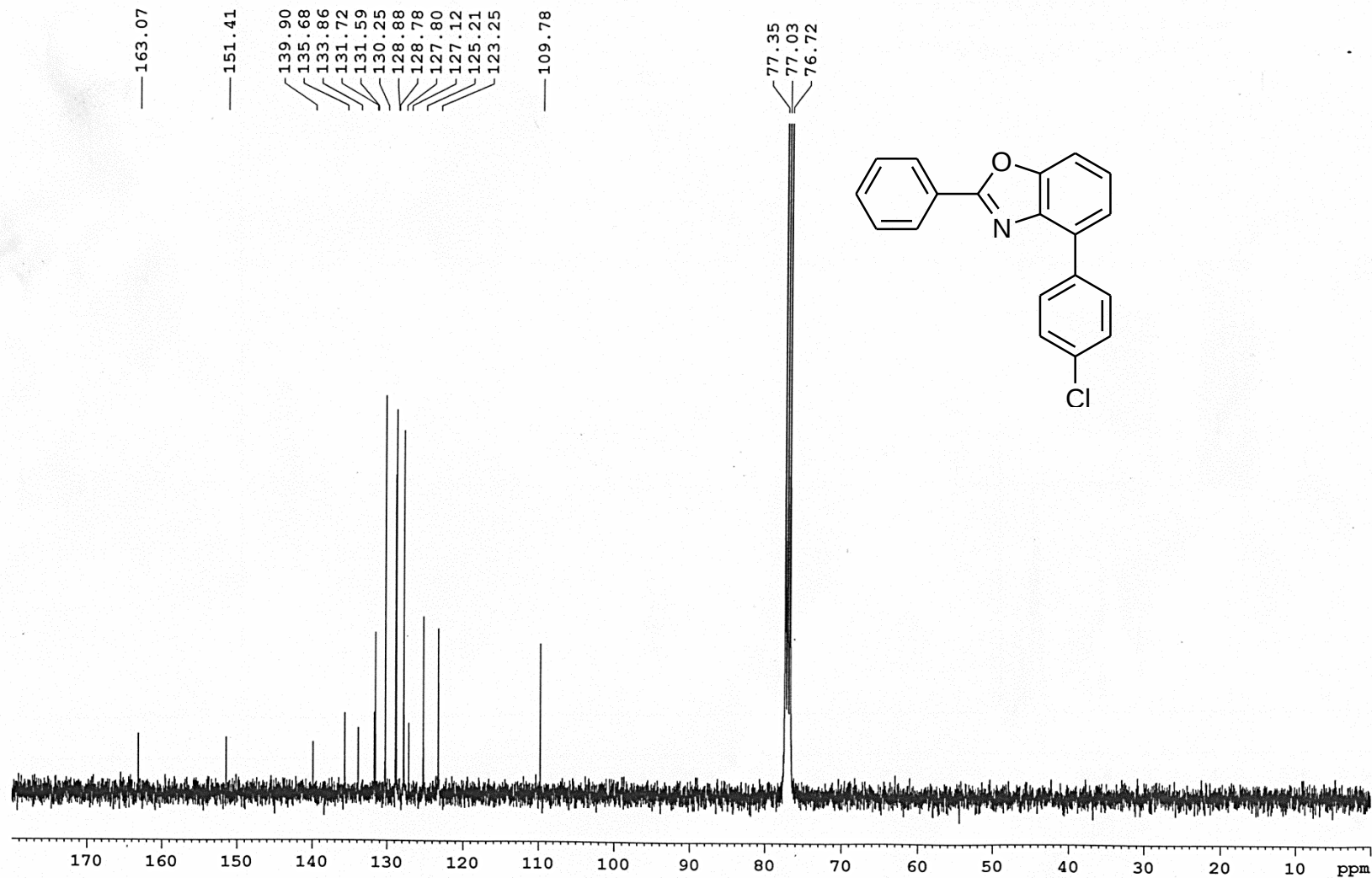
—1.660



^{13}C NMR of 4-(4-chlorophenyl)-2-phenylbenzo[d]oxazole (3ac)

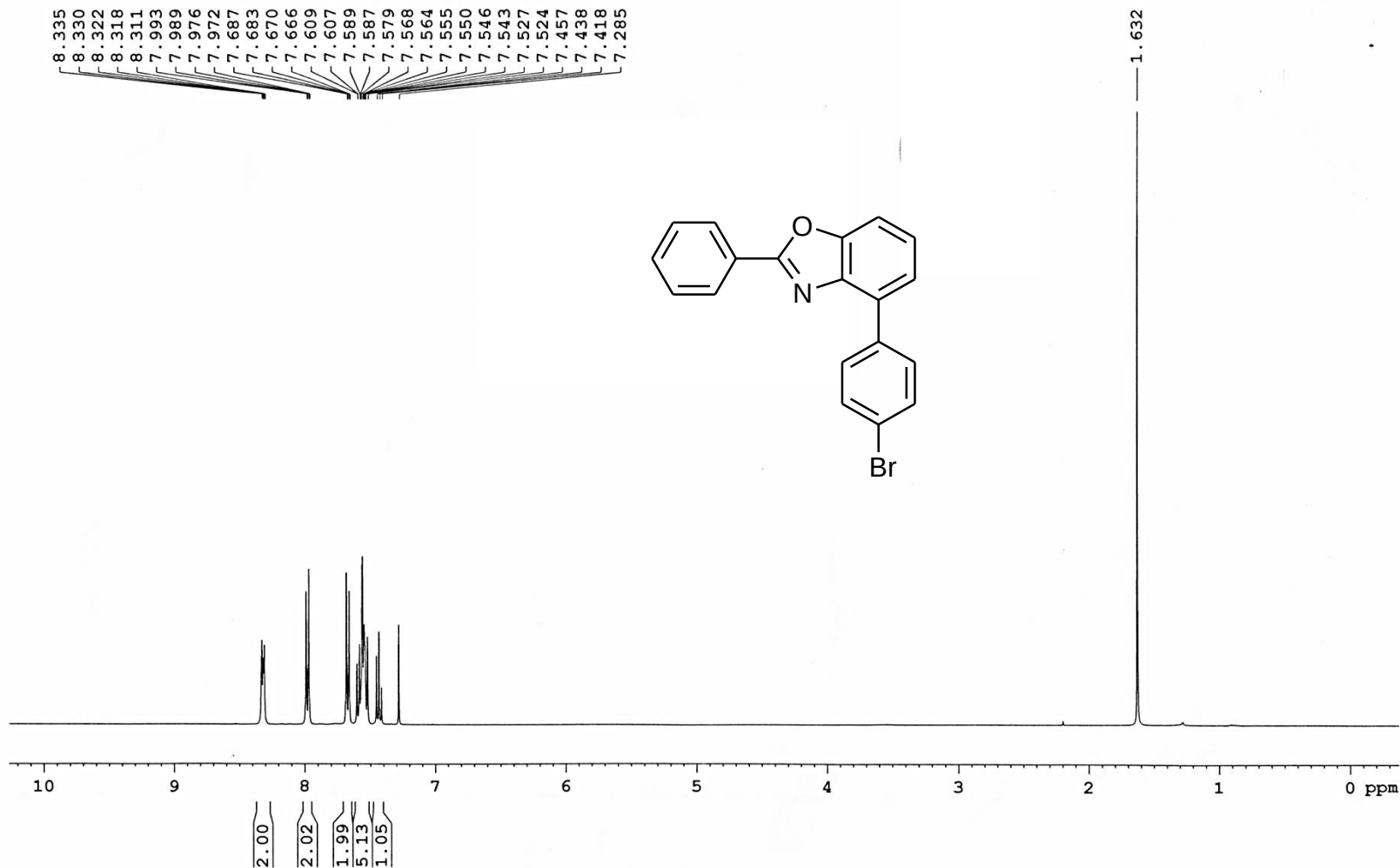
^{13}C NP-KS-Cl-I (3ac)

13.2.2020



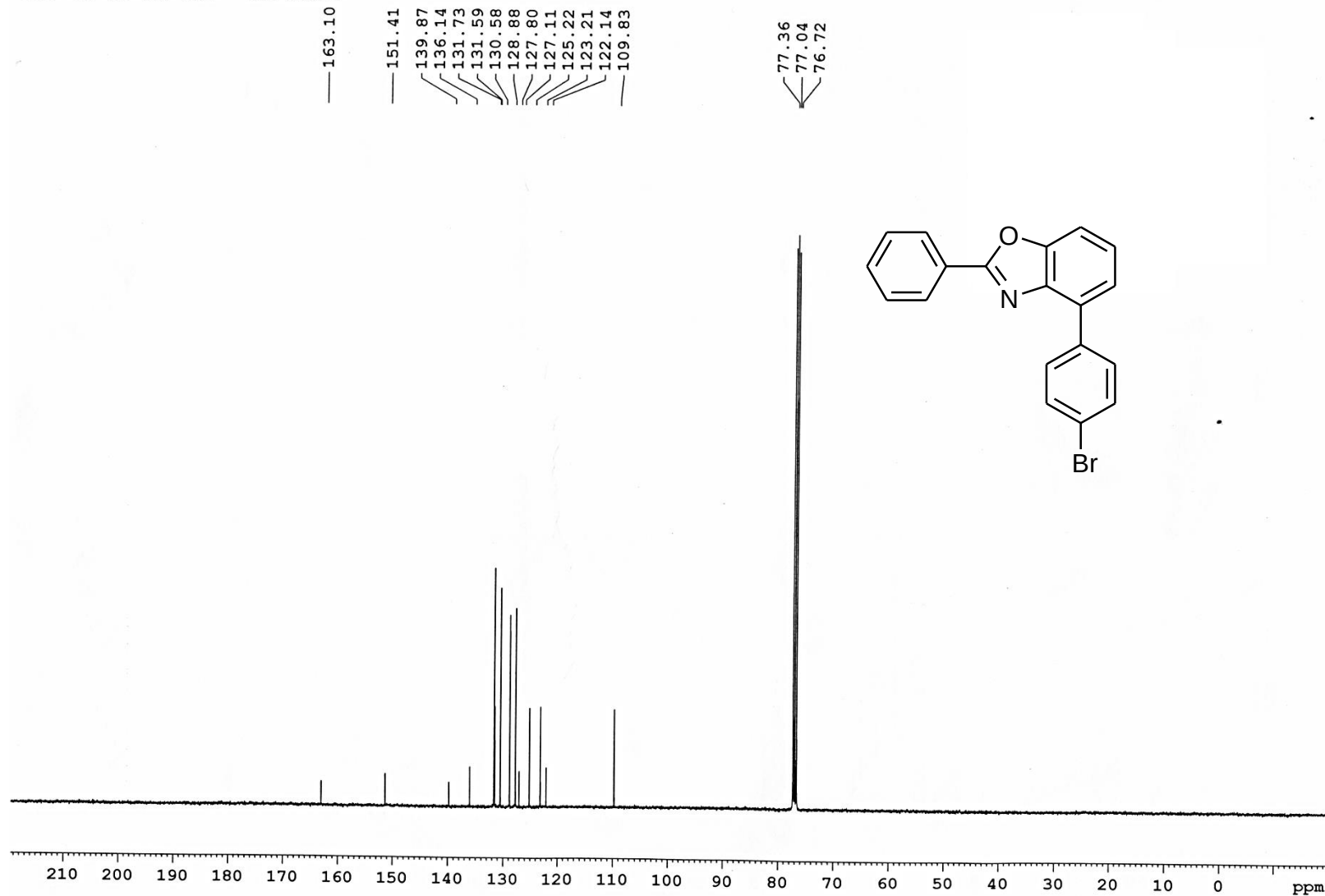
^1H NMR of (4-bromophenyl)-2-phenylbenzo[d]oxazole(3ad)

^1H of NP-KS-729 3.6.2019



¹³C NMR of (4-bromophenyl)-2-phenylbenzo[d]oxazole(3ad)

¹³C of NP-KS-729 3.6.2019

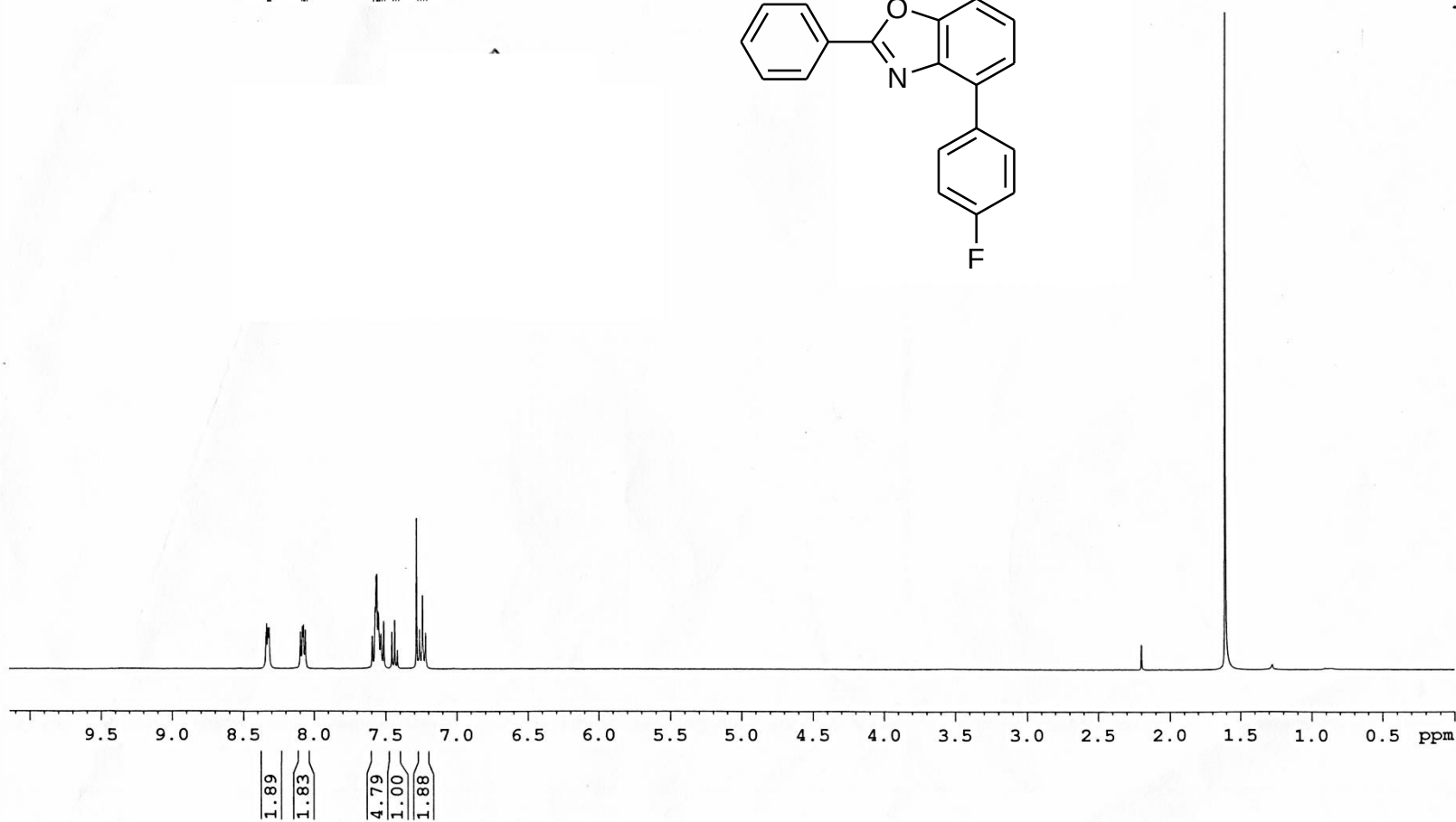
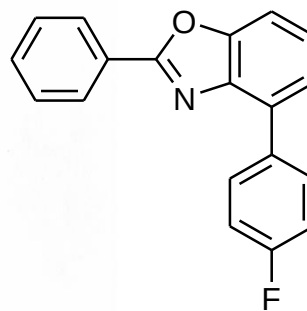


¹H NMR of 4-(4-fluorophenyl)-2-phenylbenzo[d]oxazole (3ae)

¹H of NP-KS-741

30.7.2019

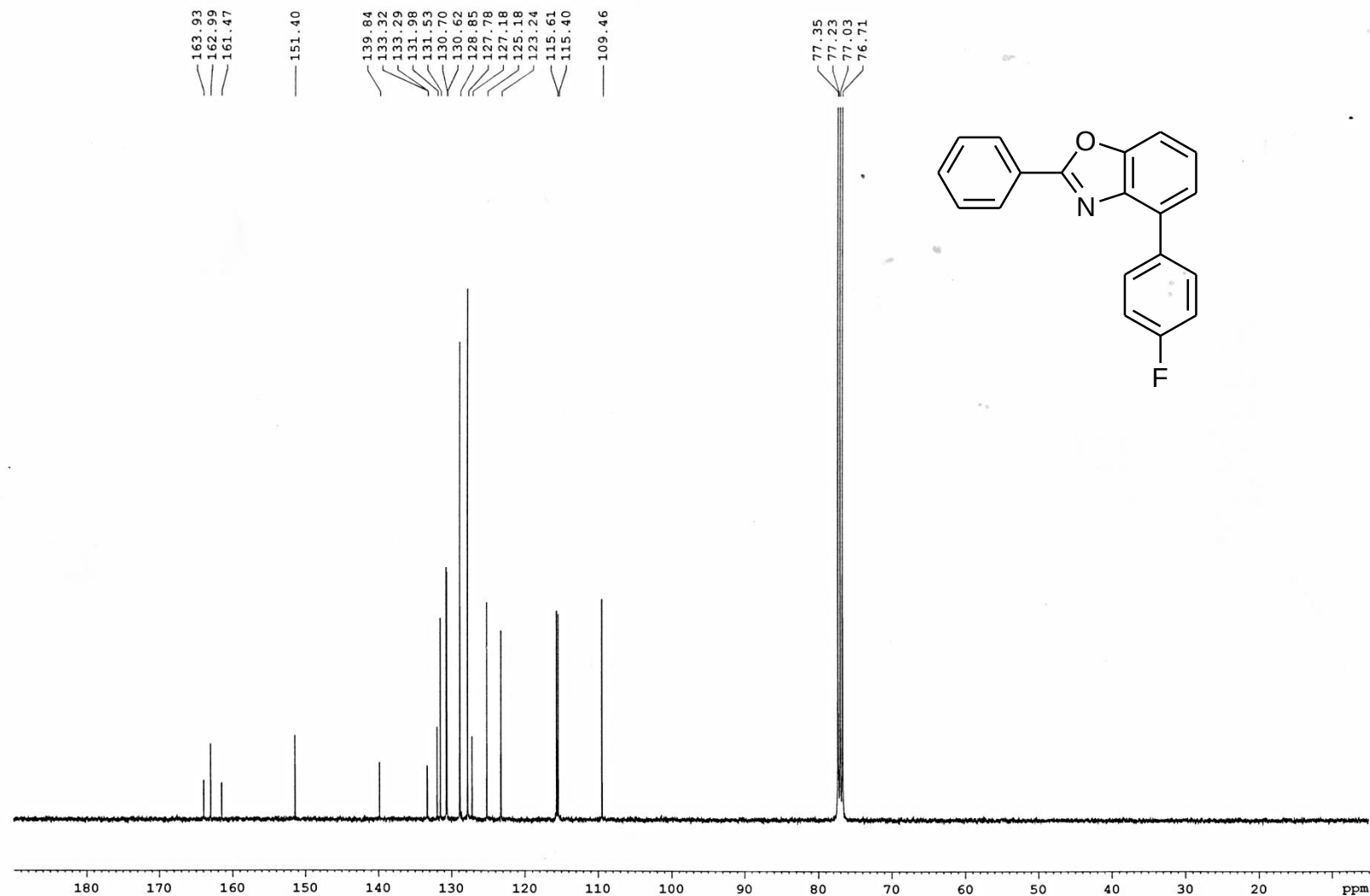
8.340
8.335
8.326
8.316
8.098
8.084
8.076
8.062
7.595
7.573
7.567
7.563
7.554
7.550
7.535
7.516
7.458
7.438
7.418
7.285
7.264
7.242
7.221



^{13}C NMR of 4-(4-fluorophenyl)-2-phenylbenzo[d]oxazole (3ae)

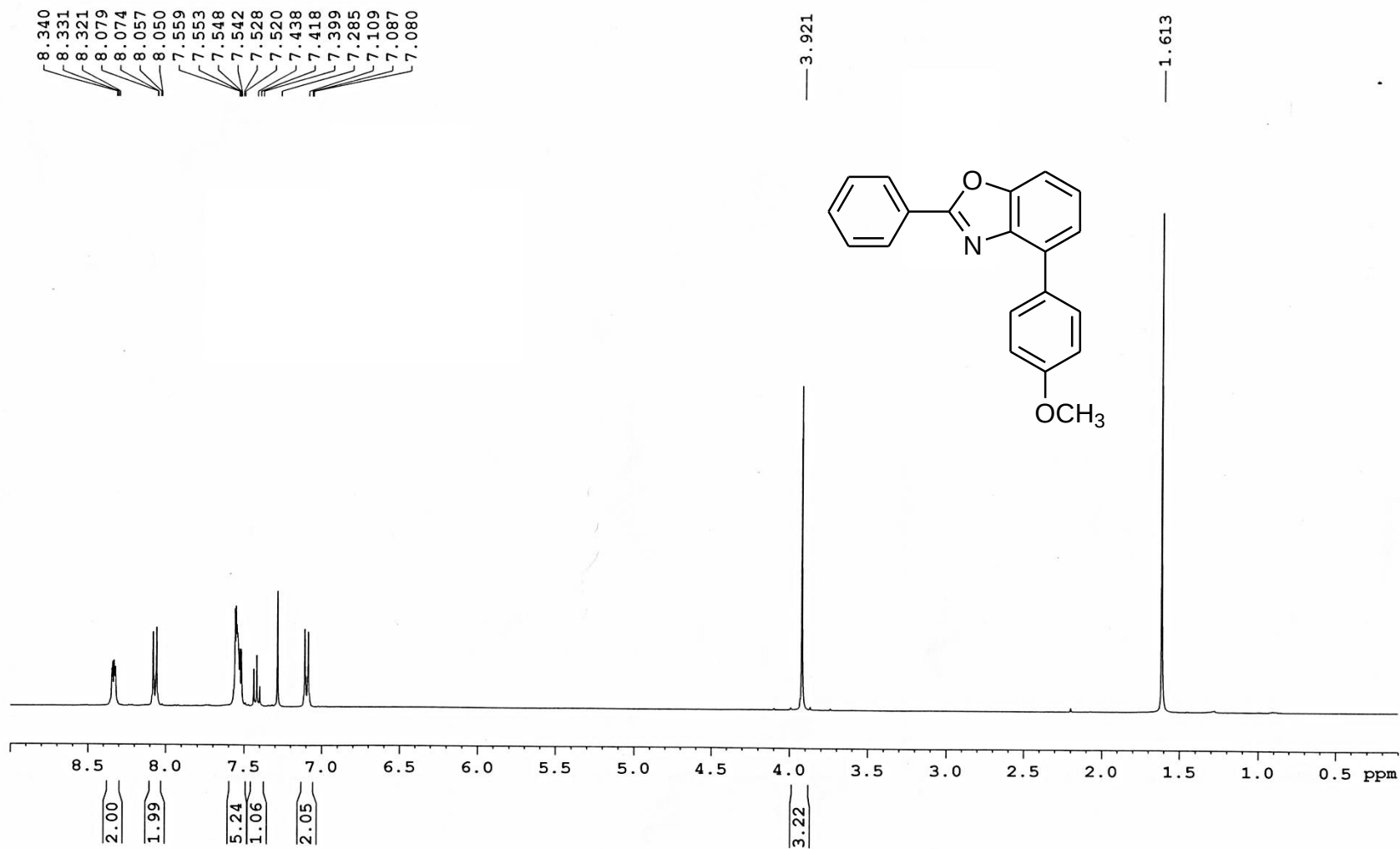
^{13}C of NP-KS-F (pure)

1.12.2019



¹H NMR of 4-(4-methoxyphenyl)-2-phenylbenzo[d]oxazole (3af)

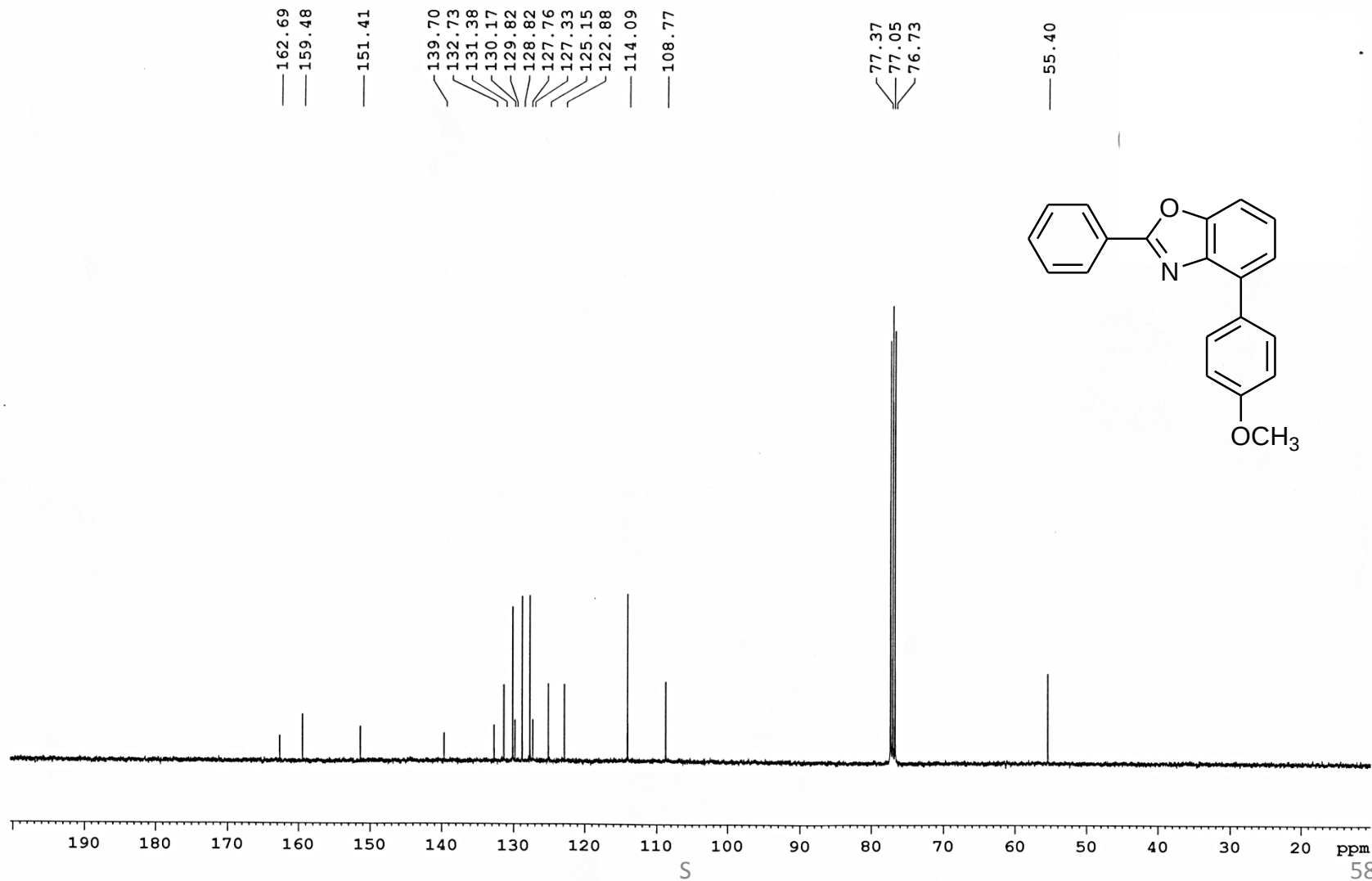
¹H of NP-KS-728 3.6.2019



^{13}C NMR of 4-(4-methoxyphenyl)-2-phenylbenzo[d]oxazole (3af)

^{13}C of NP-KS-728

2.7.2019

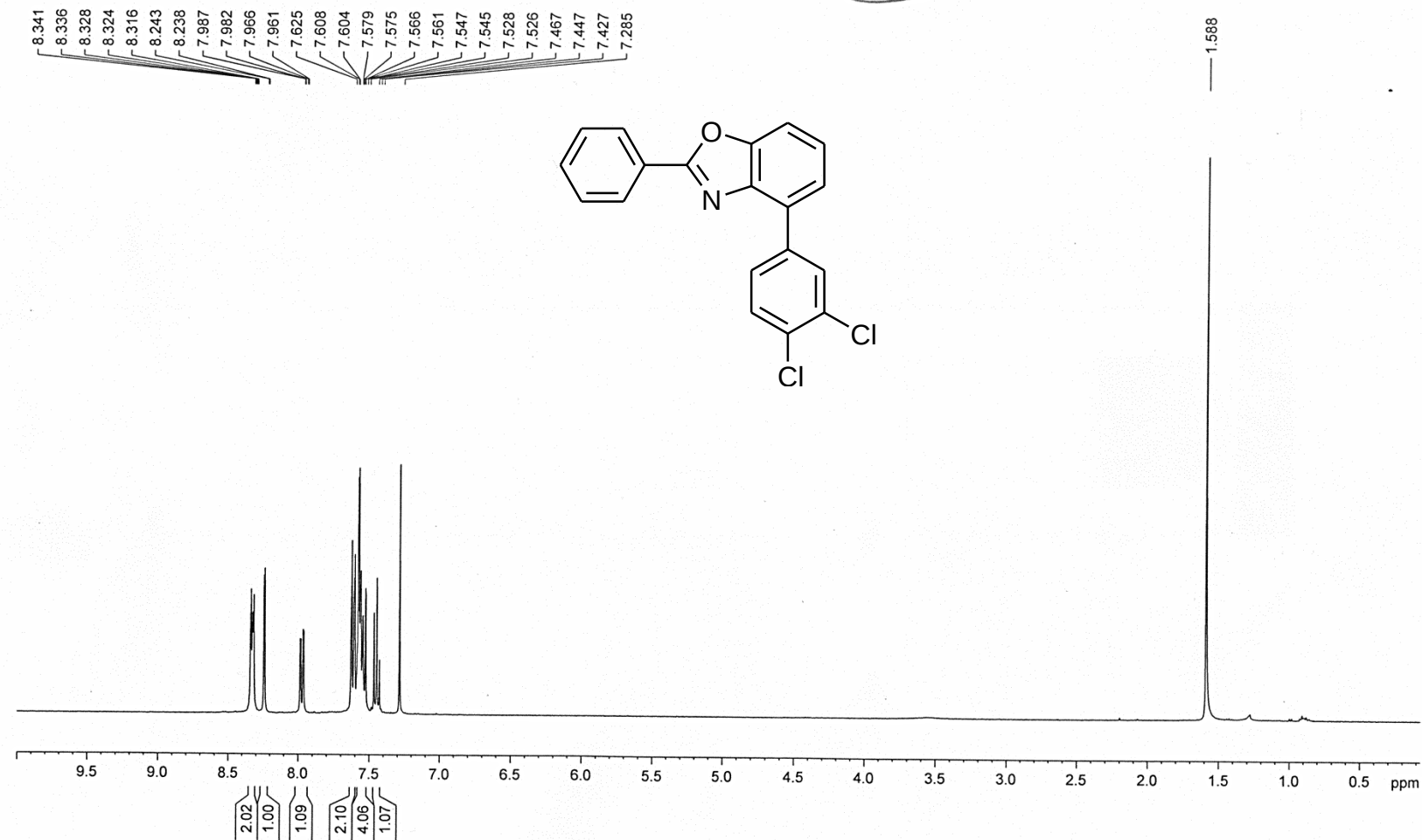


^1H NMR of 4-(3, 4- Dichloro - phenyl)-2-phenylbenzo[d]oxazole(3ag)

^1H of NP-KS-731

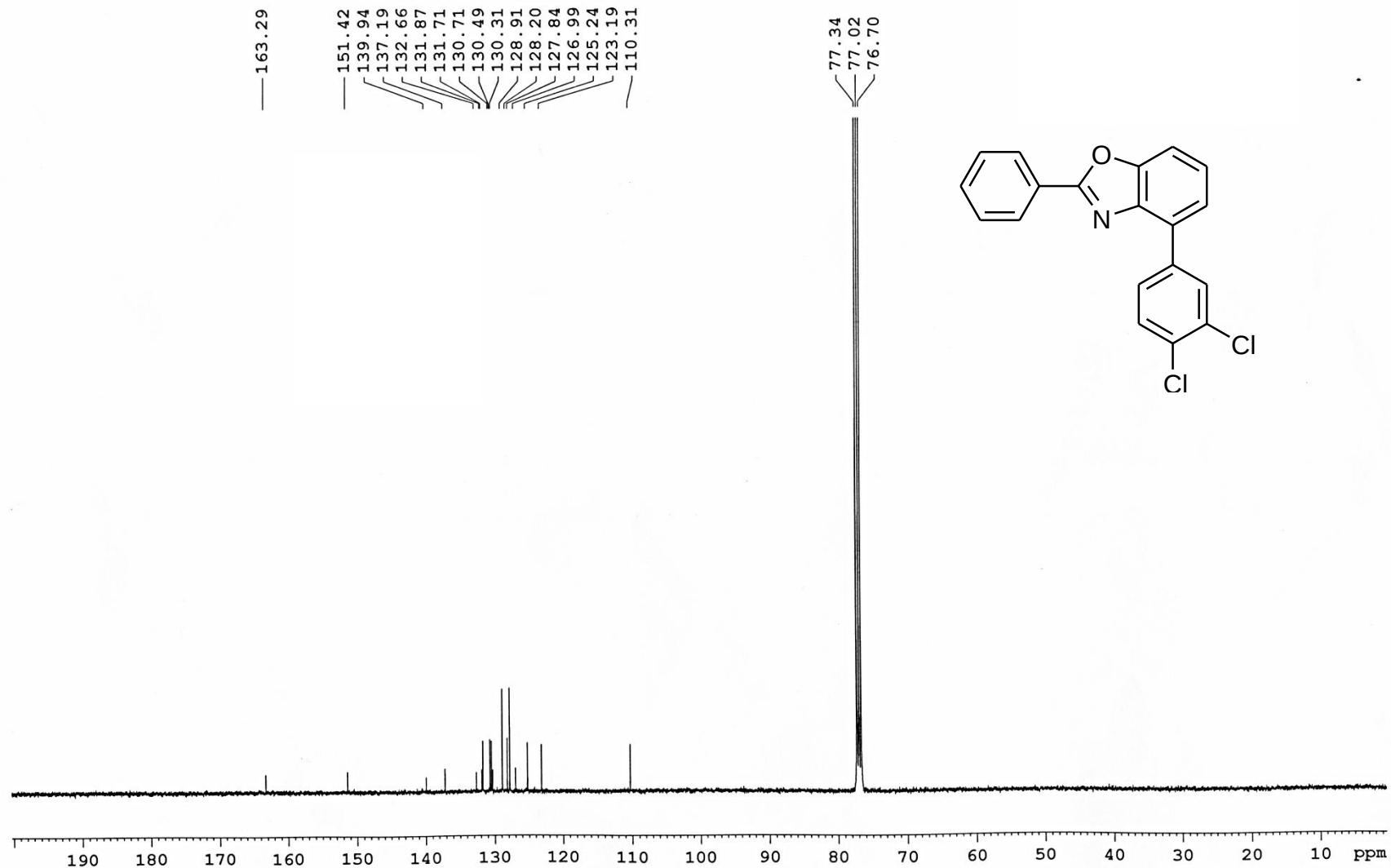
15.7.2019

3ag



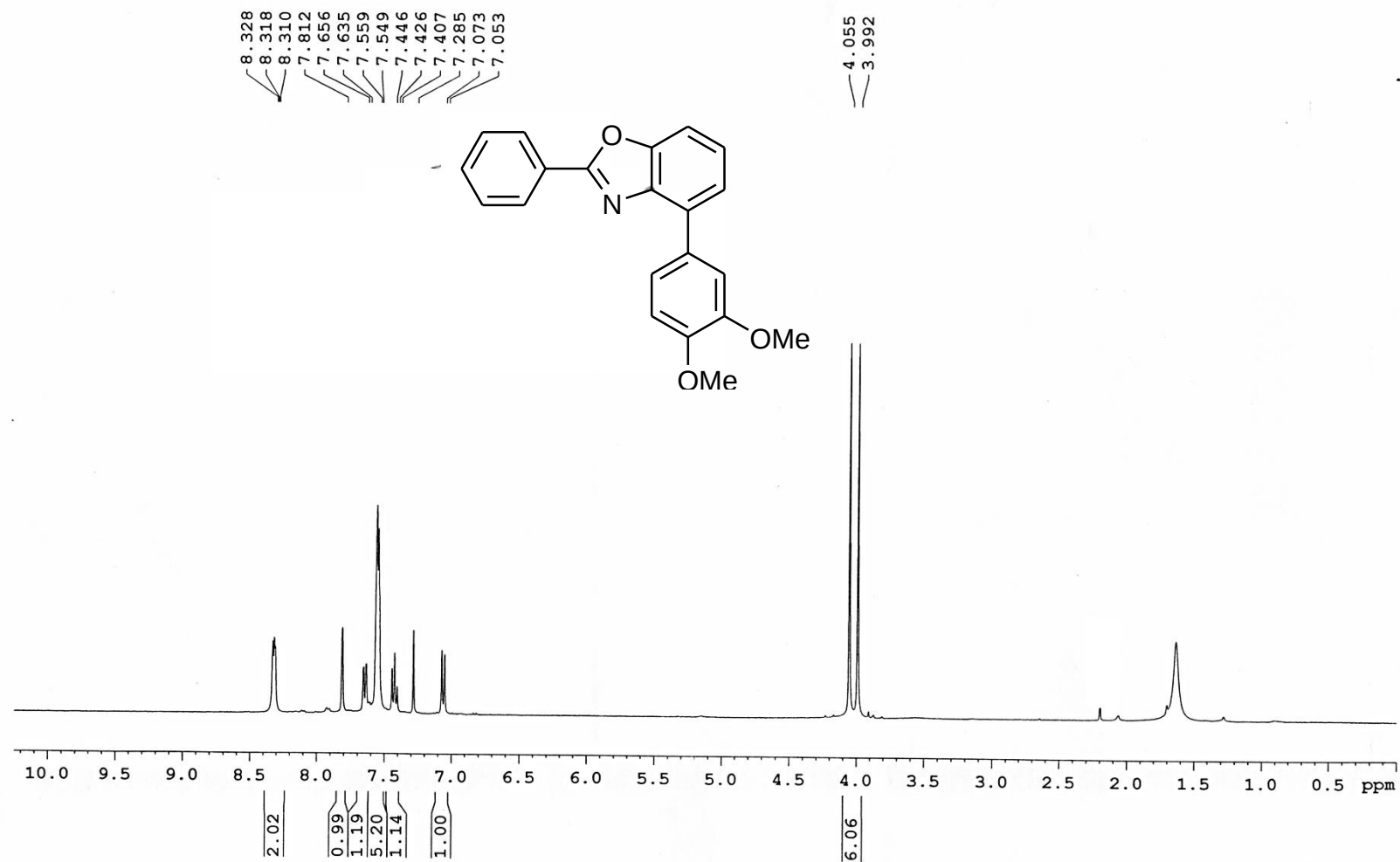
¹³C NMR of 4-(3, 4- Dichloro - phenyl)-2-phenylbenzo[d]oxazole(3ag)

¹³C of NP-KS-731 12.7.2019



¹H NMR of 4-(3,4-dimethoxyphenyl)-2-phenylbenzo[d]oxazole(3ah)

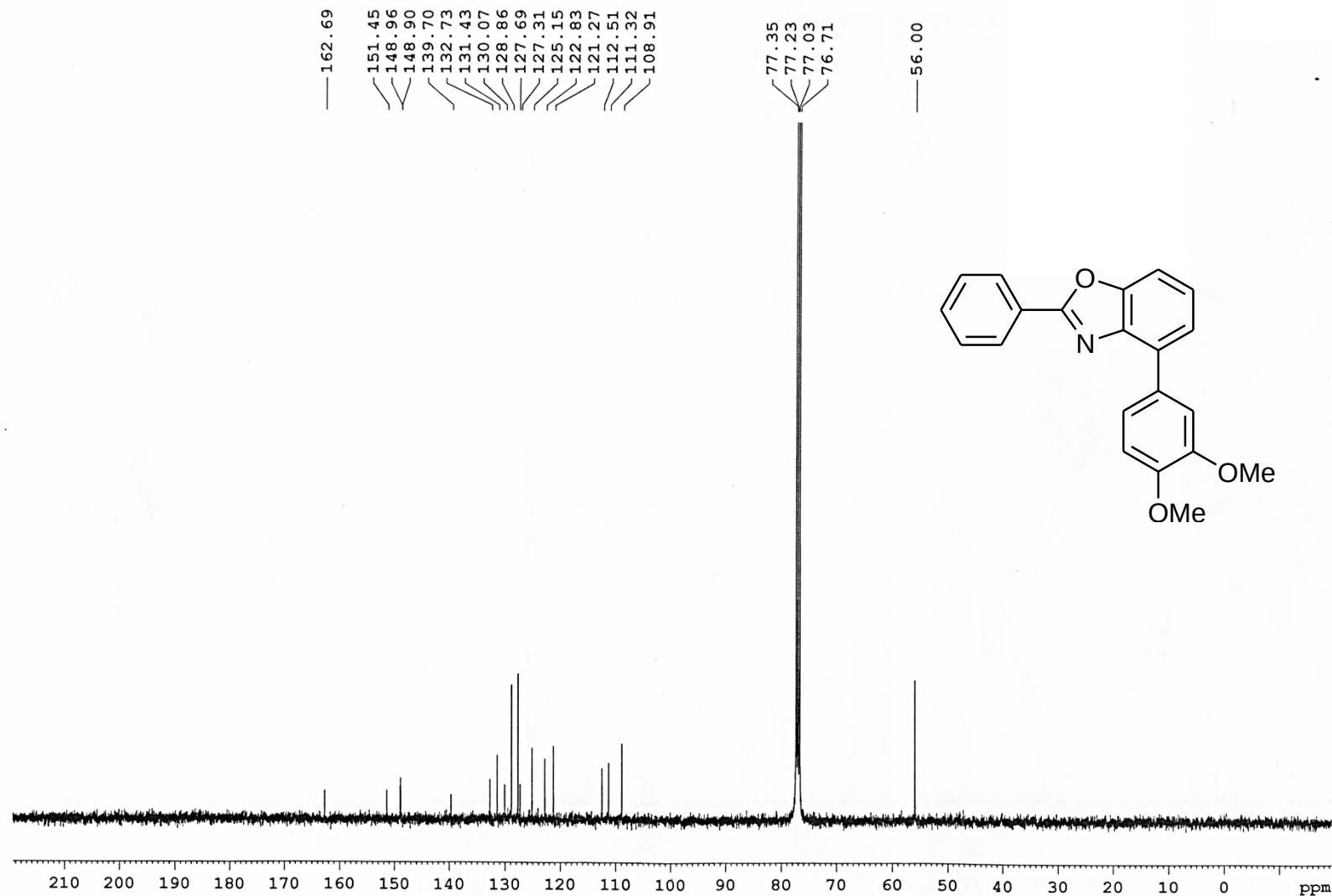
¹H of NP-KS-808 5.11.2019



^{13}C NMR of 4-(3,4-dimethoxyphenyl)-2-phenylbenzo[d]oxazole(3ah)

^{13}C of NP-KS-808

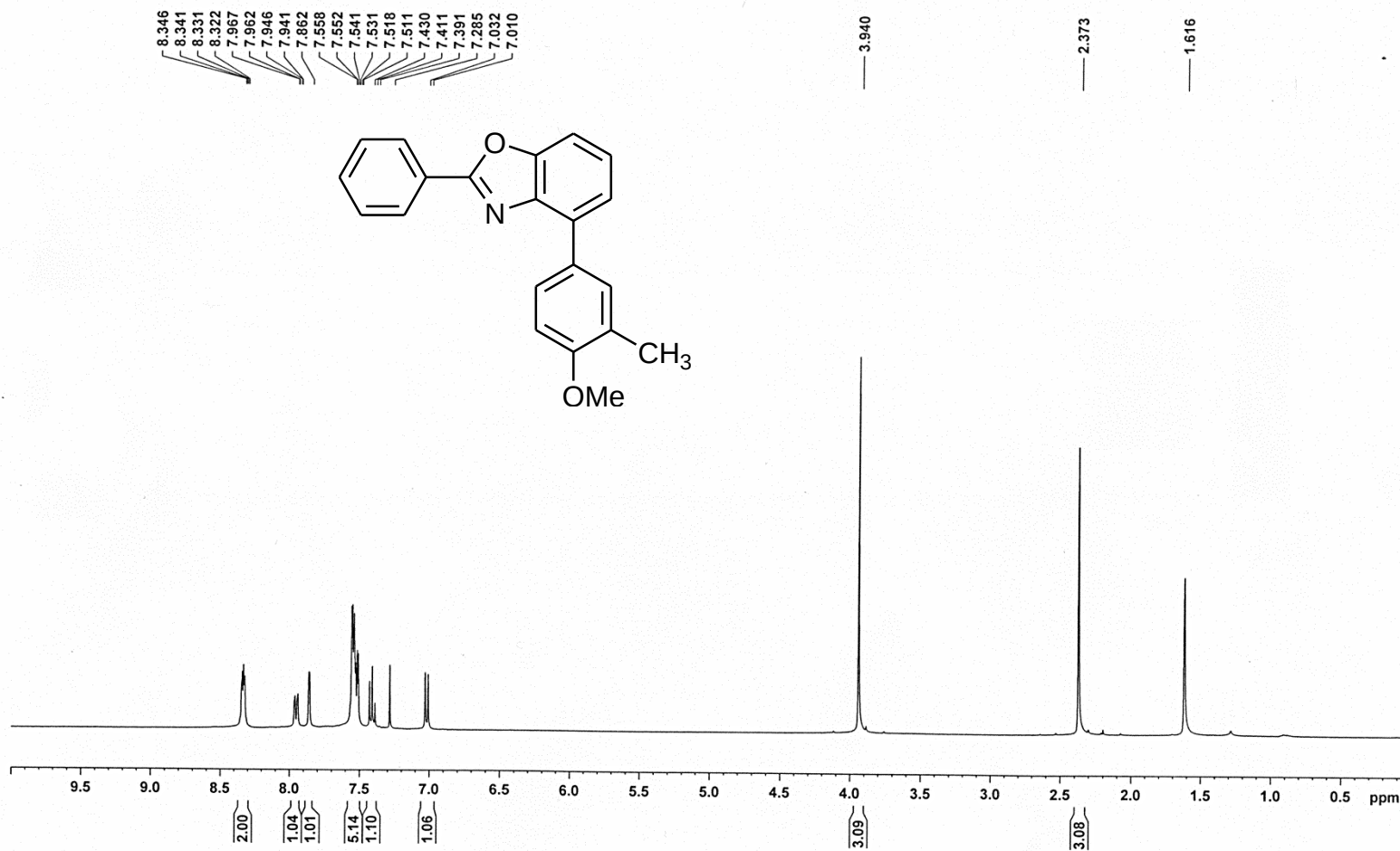
5.11.2019



^1H NMR of 4-(4-methoxy-3-methylphenyl)-2-phenylbenzo[d]oxazole(3ai)

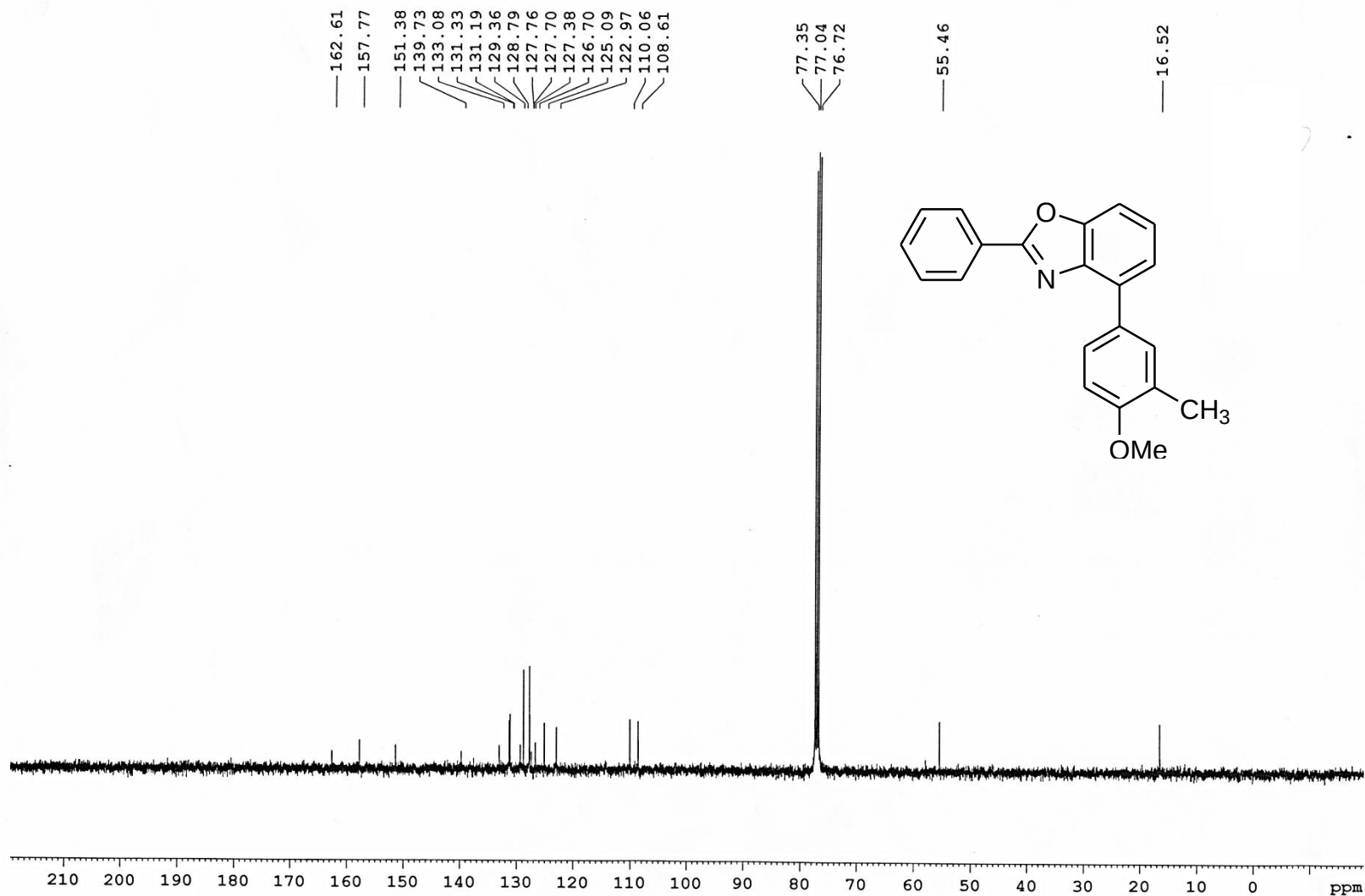
^1H of NP-KS-804 4.11.2019

3ai



¹³C NMR of 4-(4-methoxy-3-methylphenyl)-2-phenylbenzo[d]oxazole(3ai)

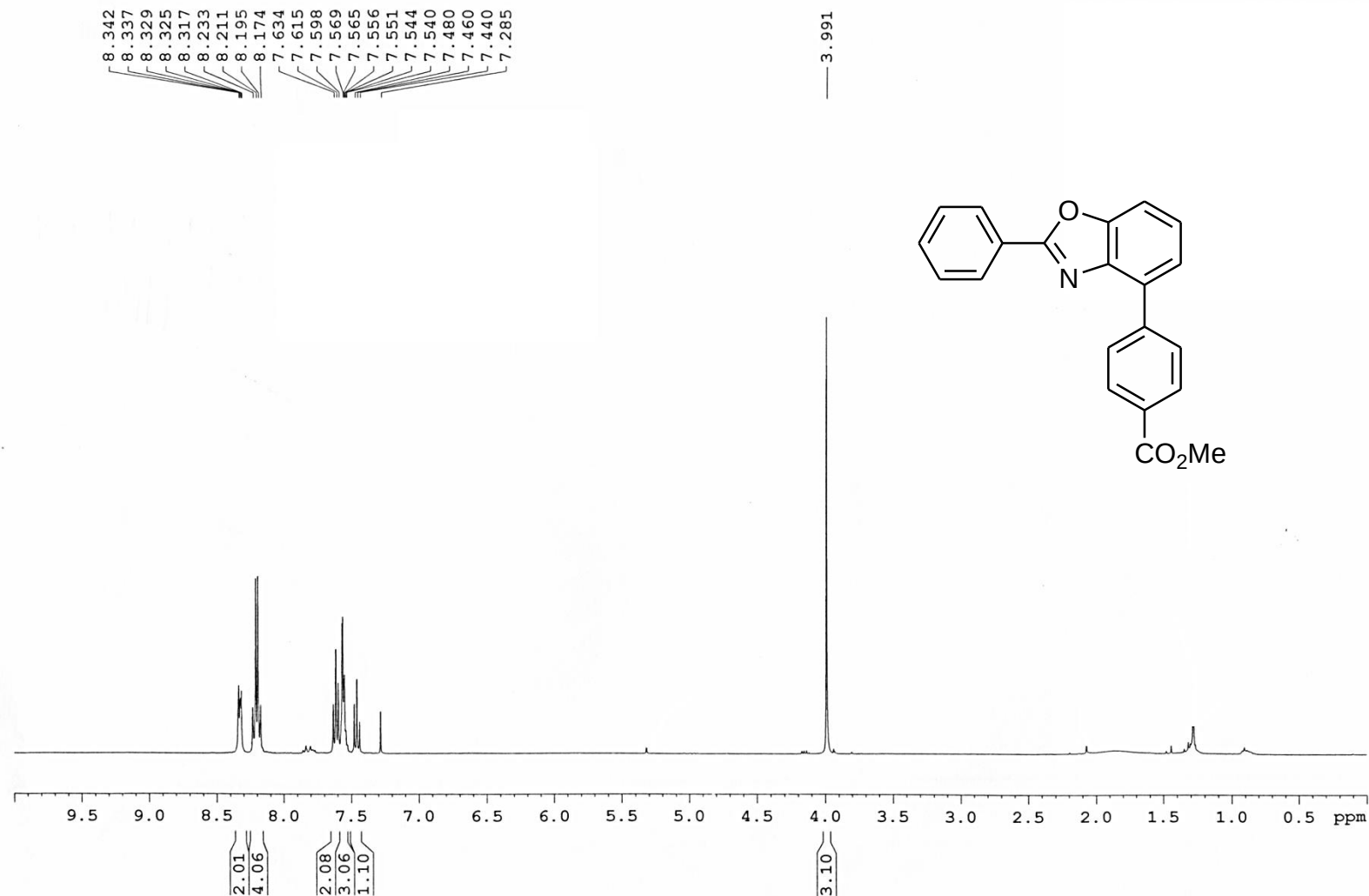
13 of NP-KS-804 4.11.2019



^1H NMR of Methyl 4-(2-phenylbenzo[d]oxazol-4-yl)benzoate (3aj)

^1H of NP-KS-774

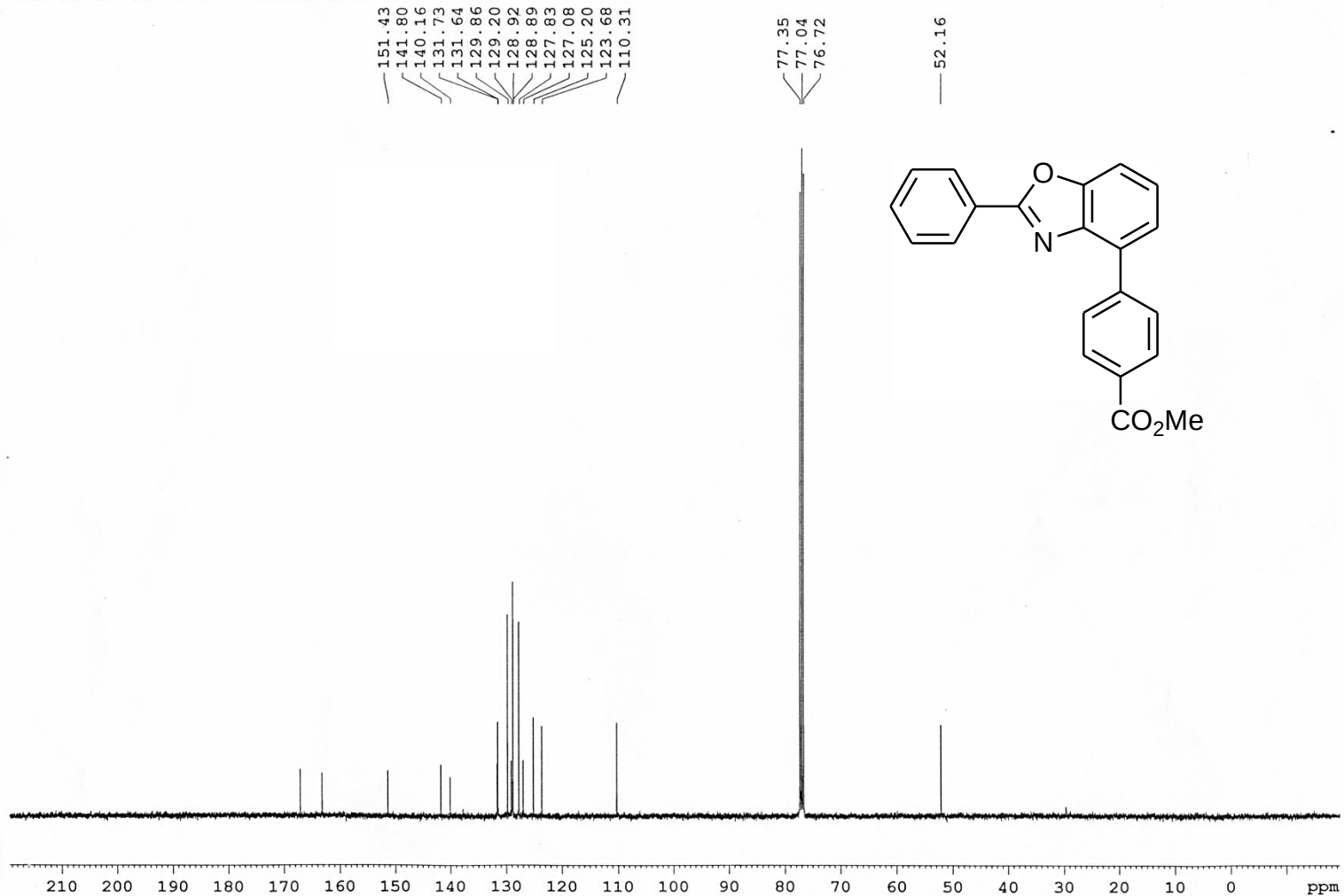
26.9.2019



¹³C NMR of Methyl 4-(2-phenylbenzo[d]oxazol-4-yl)benzoate (3aj)

13C of NP-KS-774

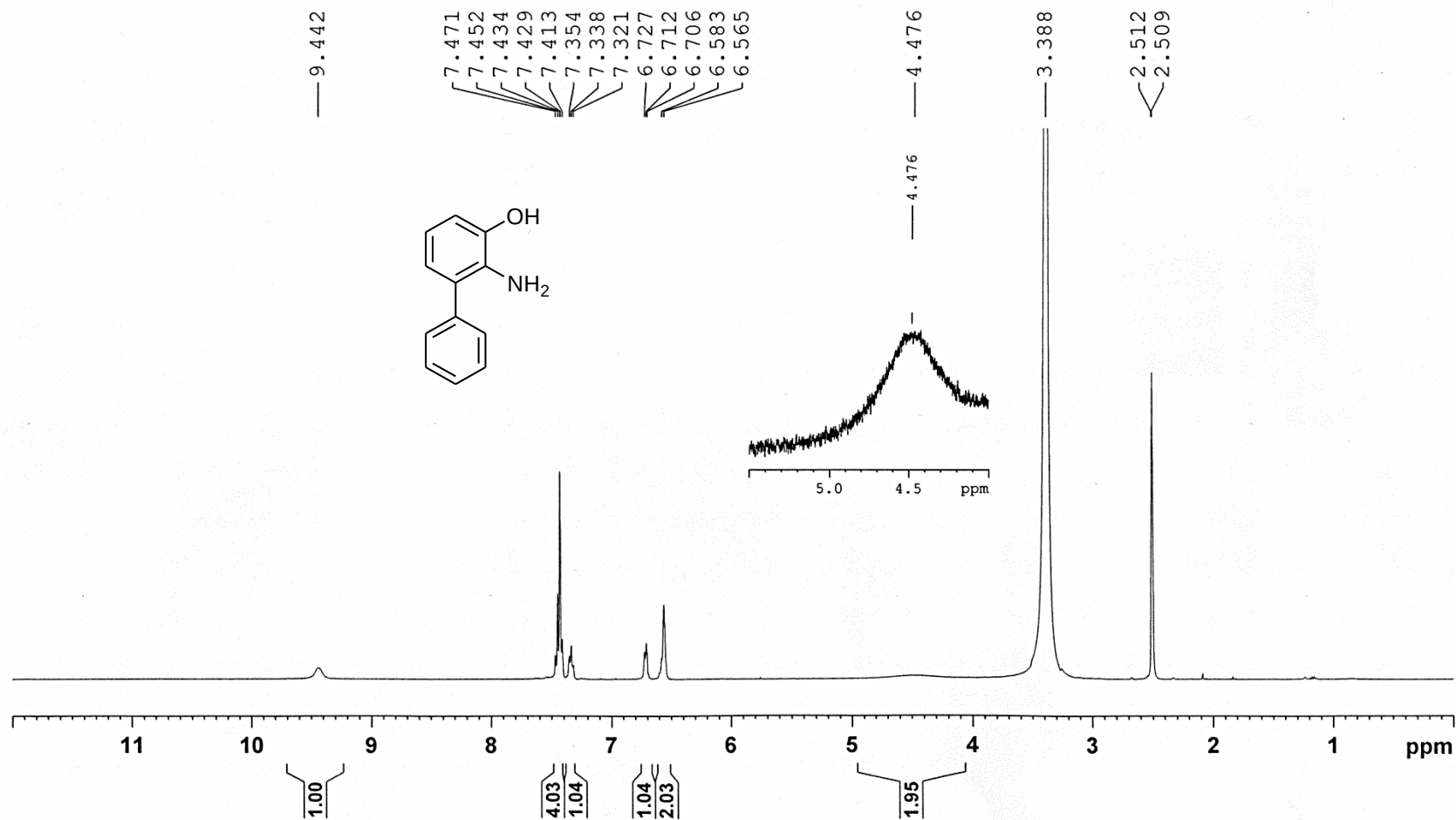
26.9.2019



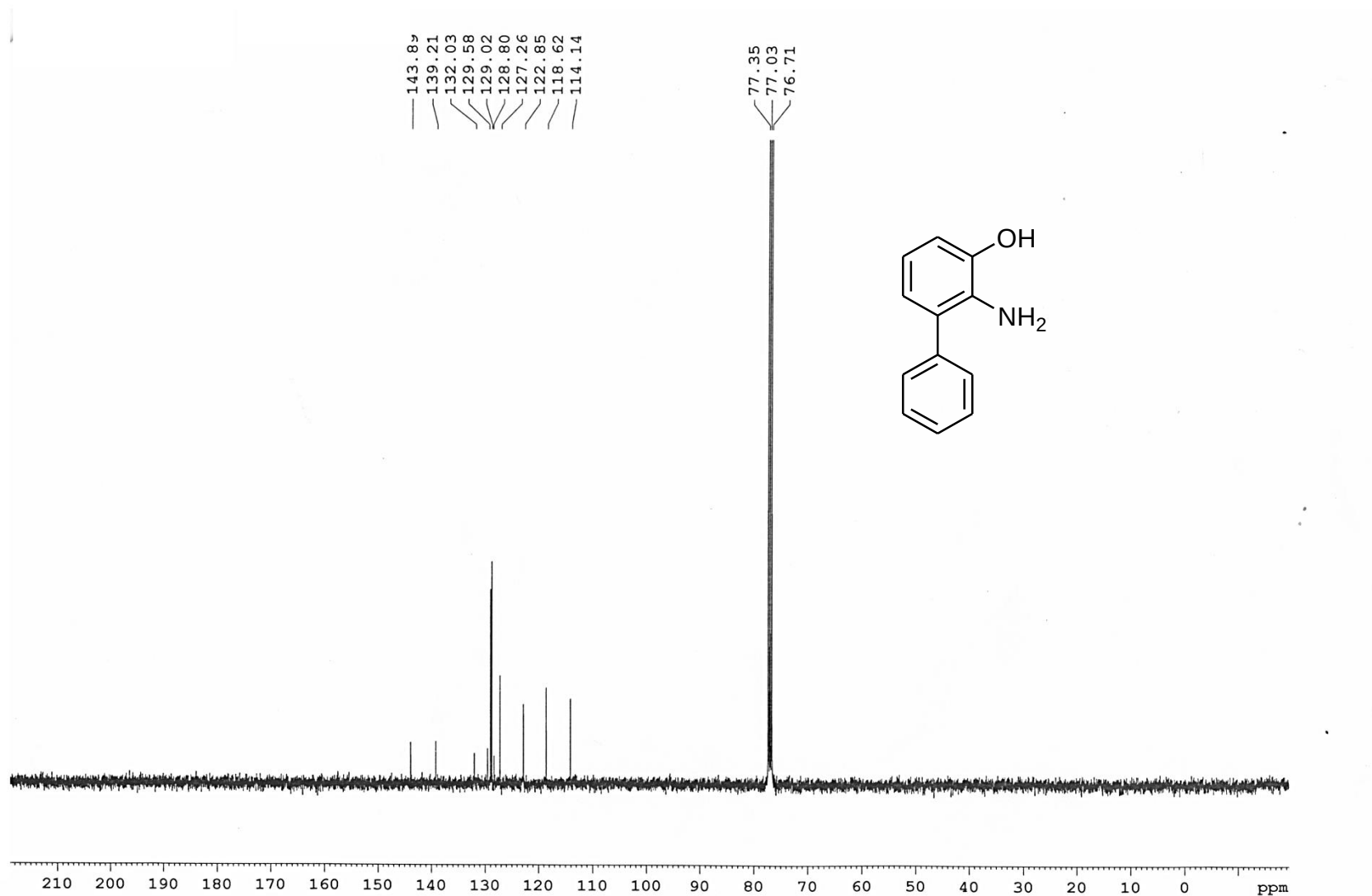
^1H NMR of 2-Amino-biphenyl-3-ol (5a)

^1H NMR of NP-KS-5a in DMSO- d_6

15.2.2020



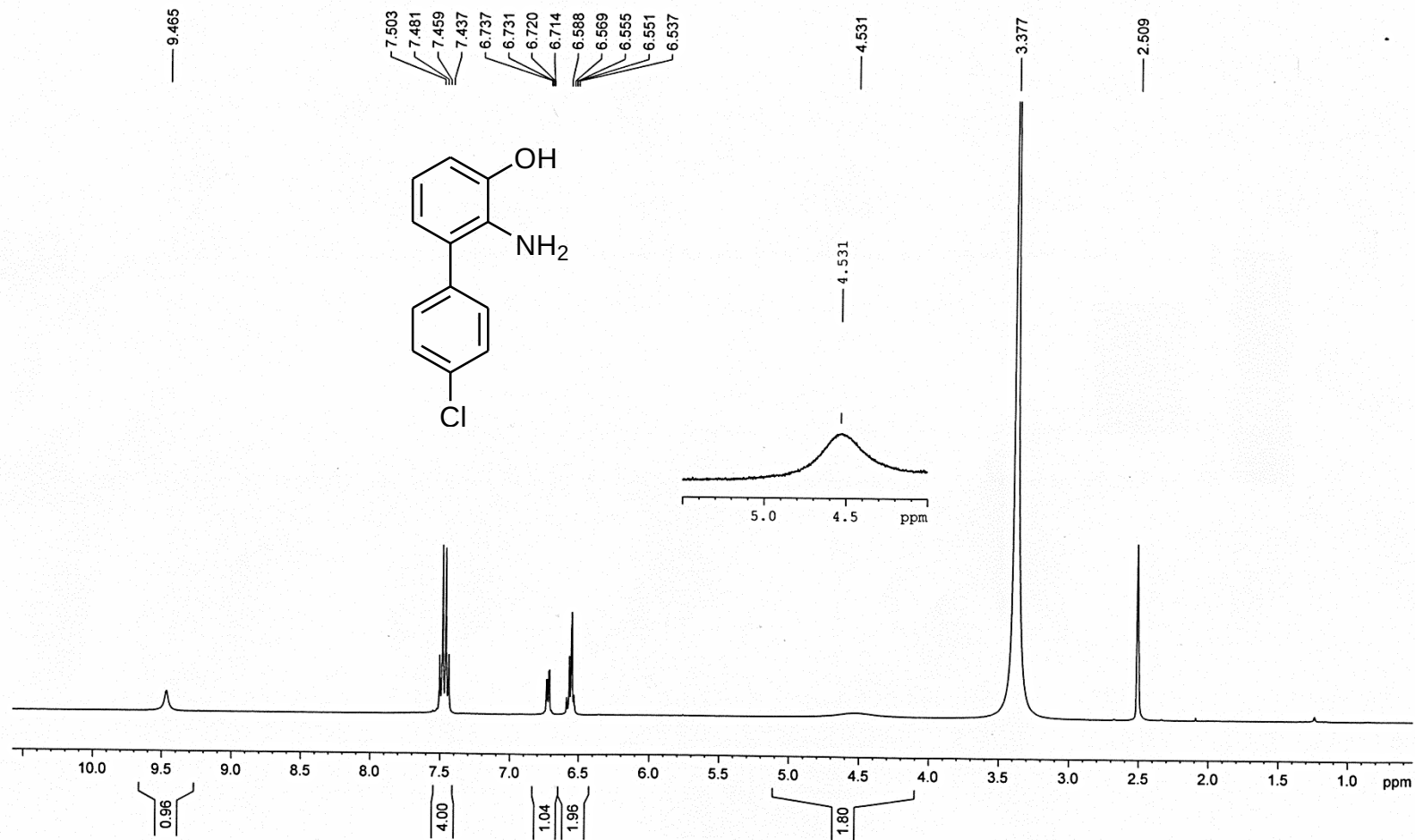
^{13}C NMR of 2-Amino-biphenyl-3-ol (5a)



^1H NMR of 2-Amino-4'-chloro-biphenyl-3-ol (5b)

NP-KS-C1 (5b) in DMSO-d₆

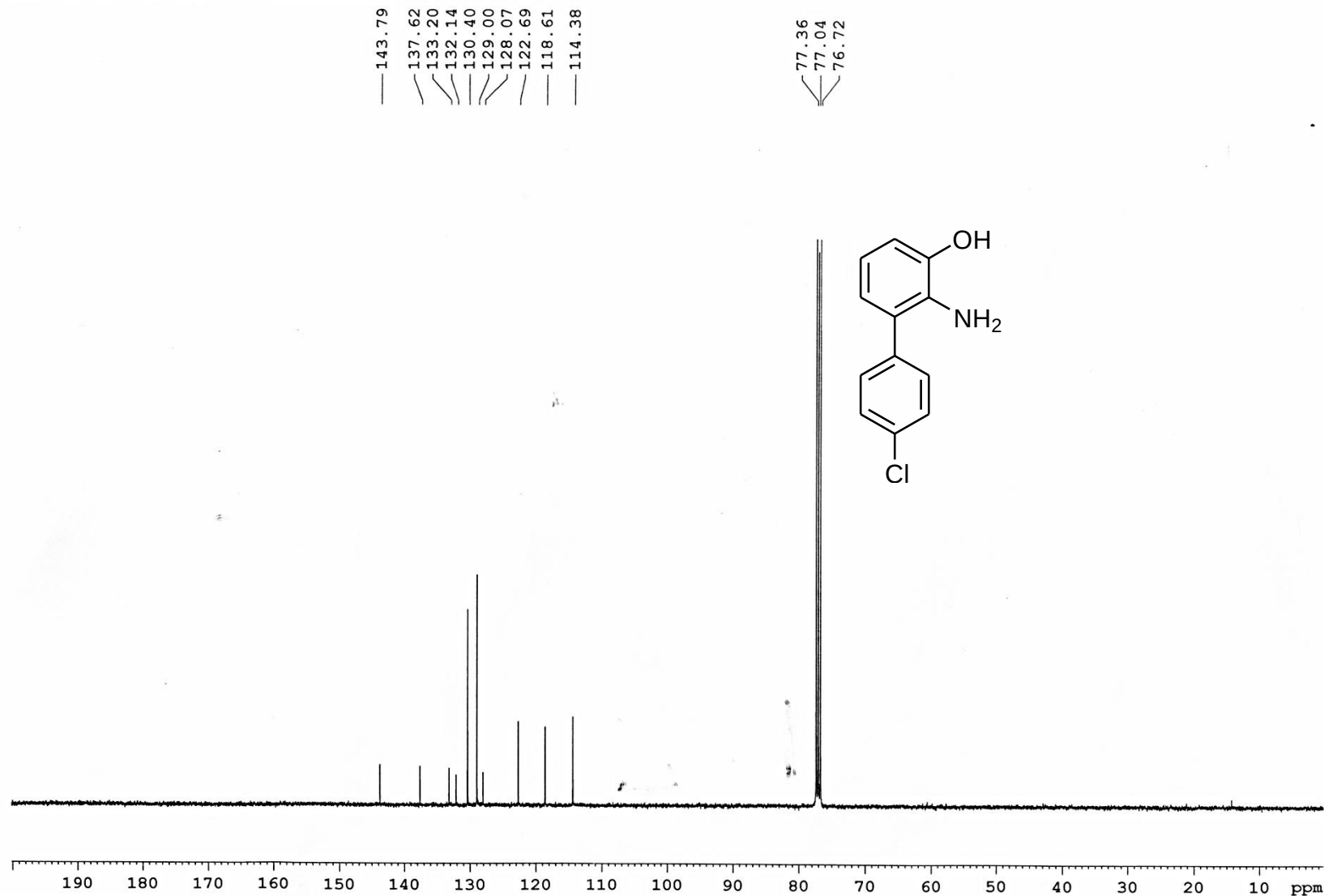
15.2.2020



¹³C NMR of 2-Amino-4'-chloro-biphenyl-3-ol (5b)

13C of NP-KS-816

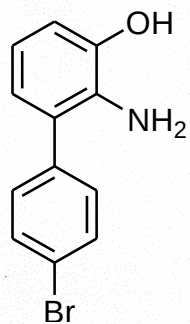
15.11.2019



^1H NMR of 2-Amino-4'-bromo-biphenyl-3-ol (5c)

^1H OF NP-KS-823 (PURE) 19.11.2019 5c

In CDCl_3

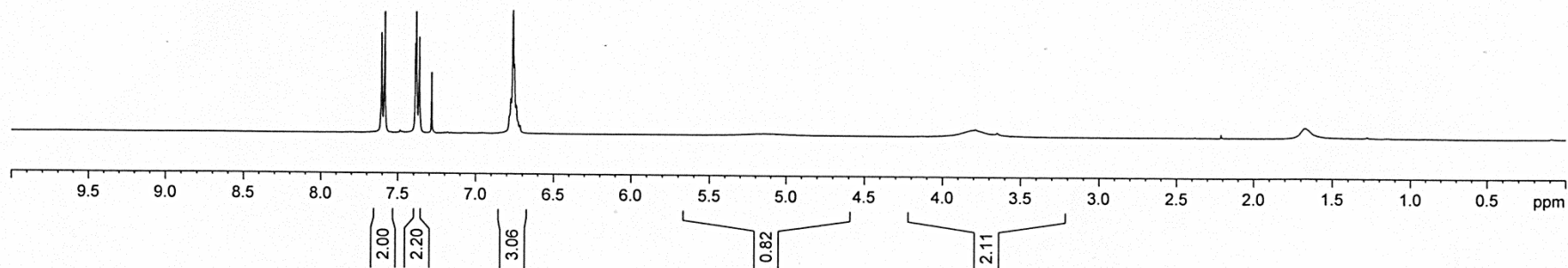
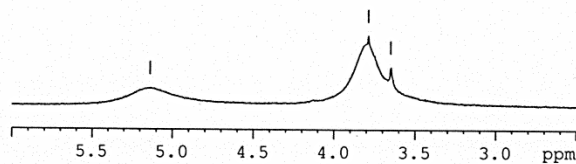


7.607
7.587
7.391
7.385
7.364
7.285
6.776
6.763
6.754
6.741

5.139

3.789
3.651

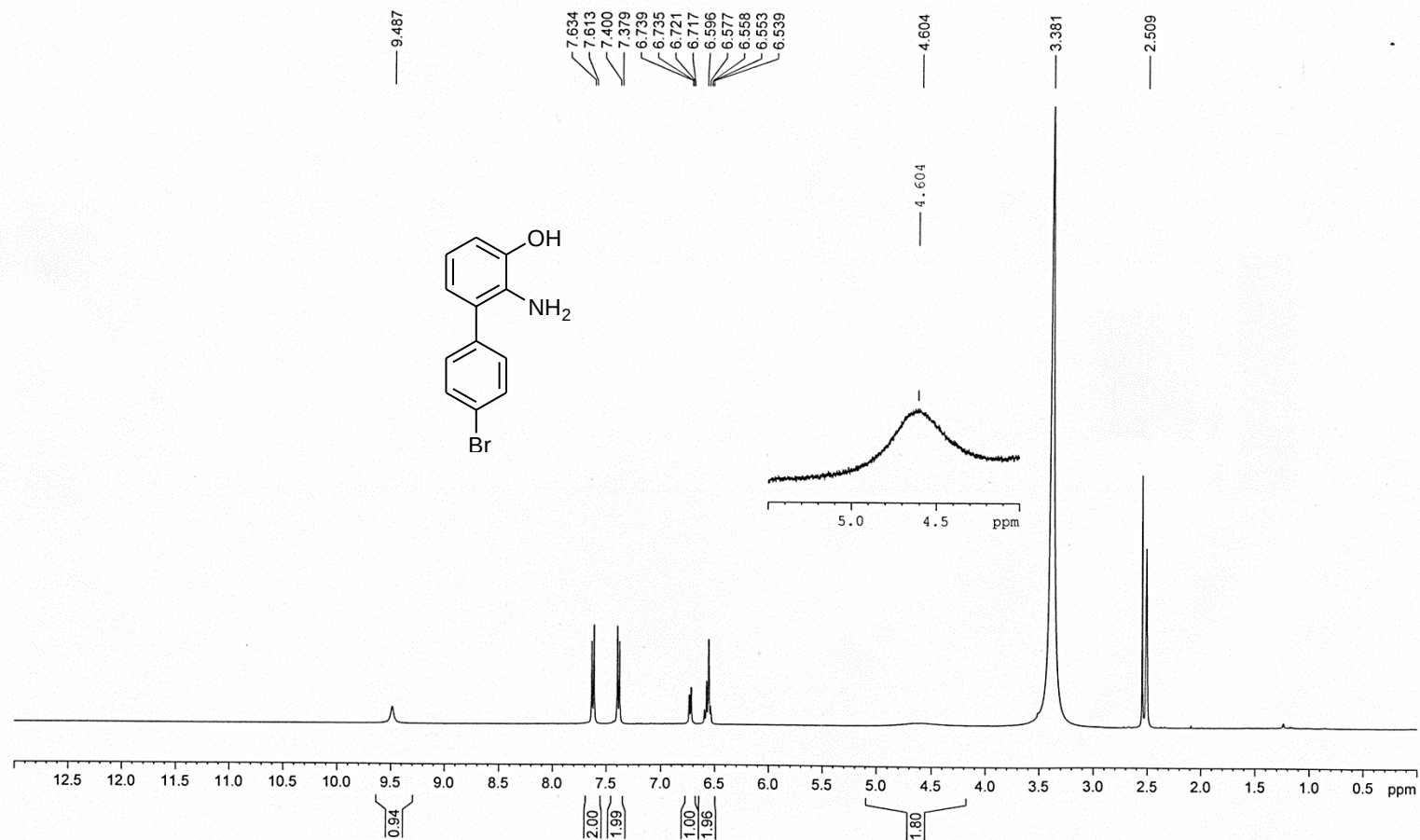
1.676



^1H NMR of 2-Amino-4'-bromo-biphenyl-3-ol (5c)

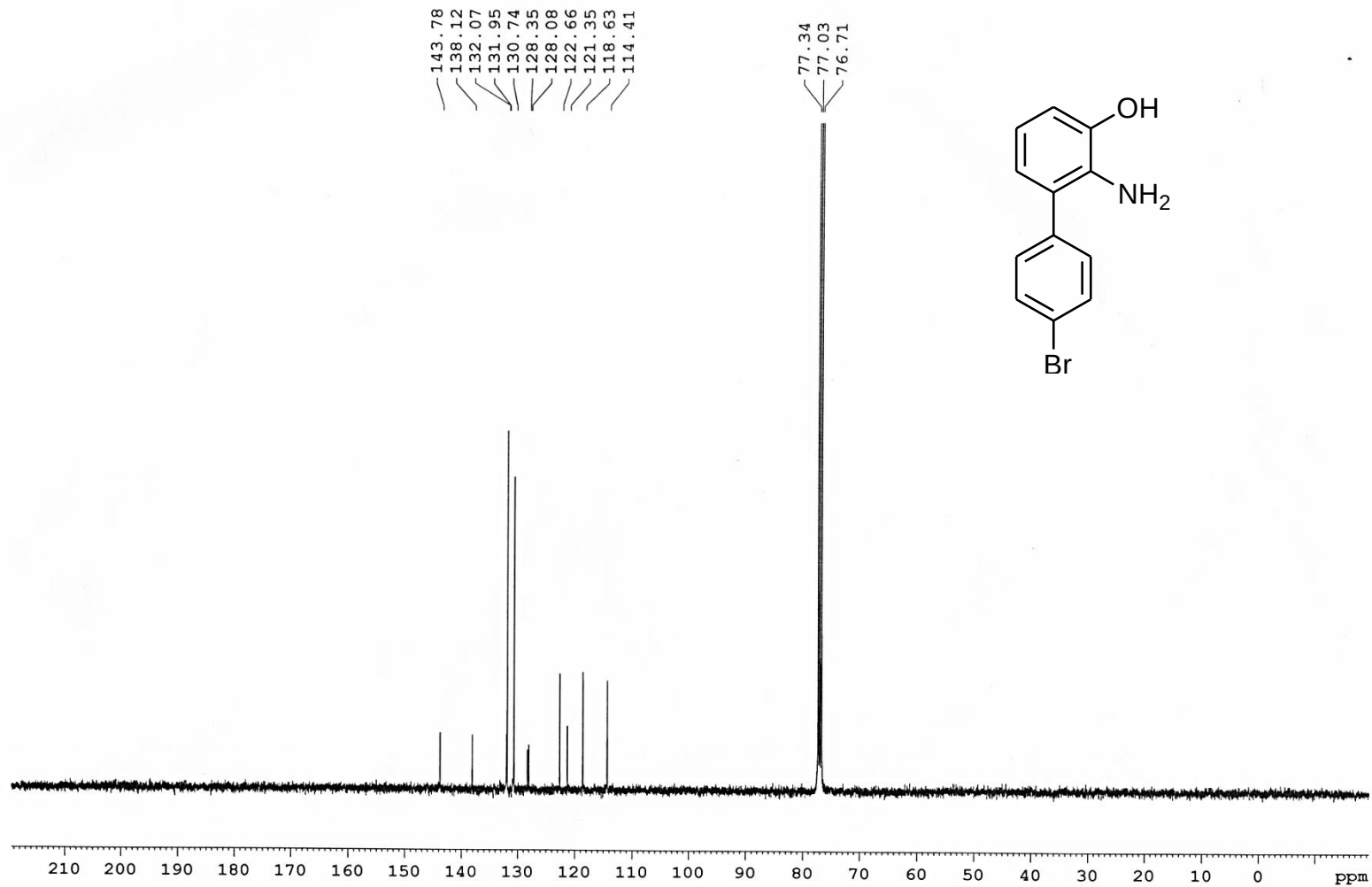
^1H NMR of NP-KS-Br-5c in DMSO- d_6

15.2.2020



¹³C NMR of 2-Amino-4'-bromo-biphenyl-3-ol (5c)

1H OF NP-KS-823 (PURE) 20.11.2019



¹H NMR of 2-Amino-4'-fluorobiphenyl-3-ol (5d)

¹H of NP-KS-F Amino

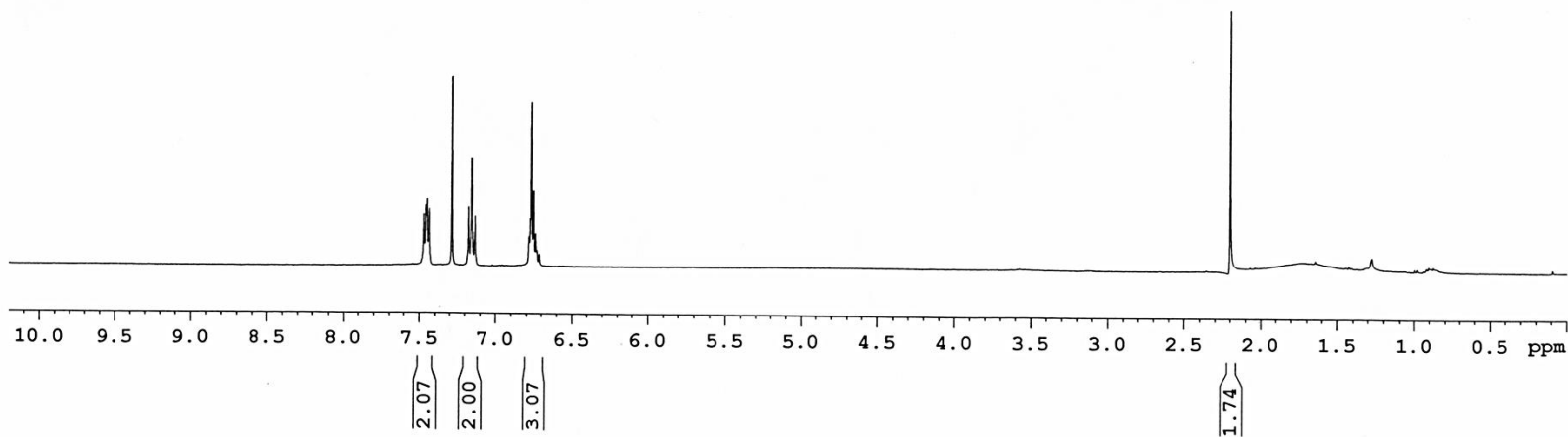
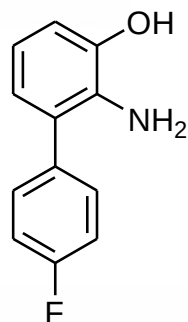
3.12.2019

7.473
7.459
7.452
7.438
7.285
7.179
7.157
7.136
6.788
6.779
6.765
6.750
6.737
6.727
6.713

— 2.201

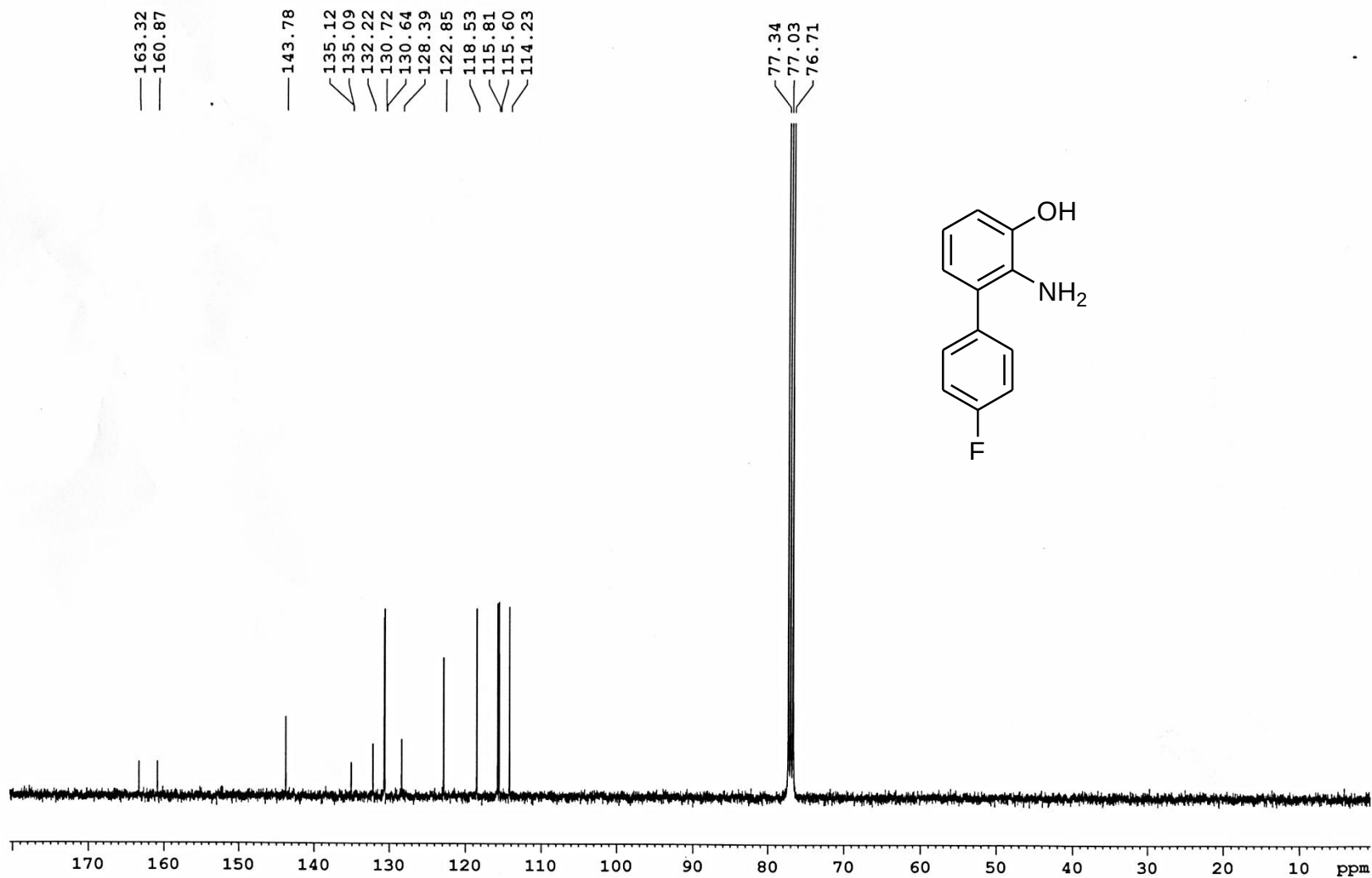
— 1.638

— 1.278



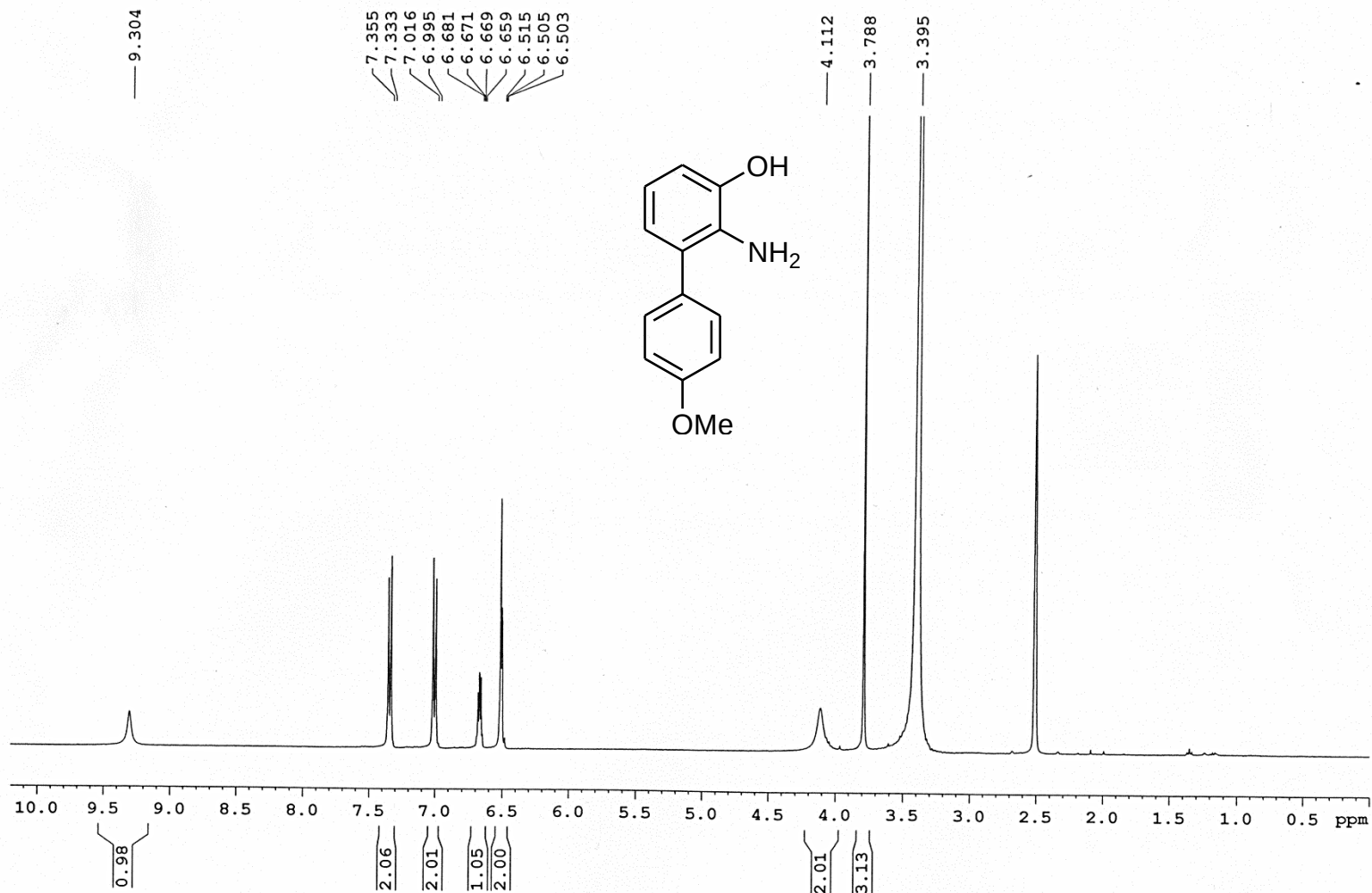
¹³C NMR of 2-Amino-4'-fluorobiphenyl-3-ol (5d)

¹³C NMR of NP-KS-F-amino 2.12.2019



^1H NMR of 2-Amino-4'-methoxy-biphenyl-3-ol (5e)

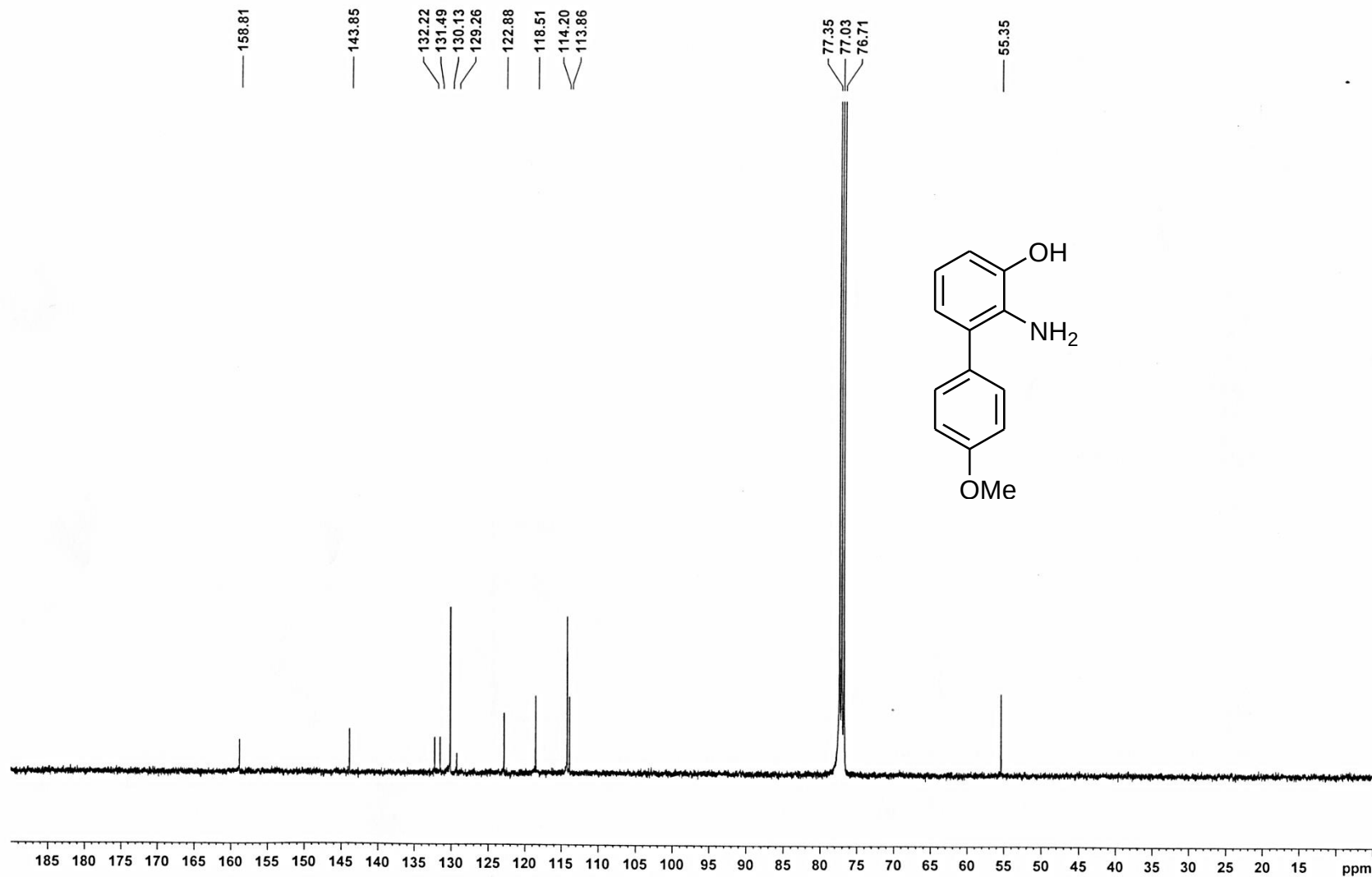
^1H of NP-KS-4oMe 14.2.2020 in DMSO-d₆



¹³C NMR of 2-Amino-4'-methoxy-biphenyl-3-ol (5e)

13C of NP-KS-813-repeat

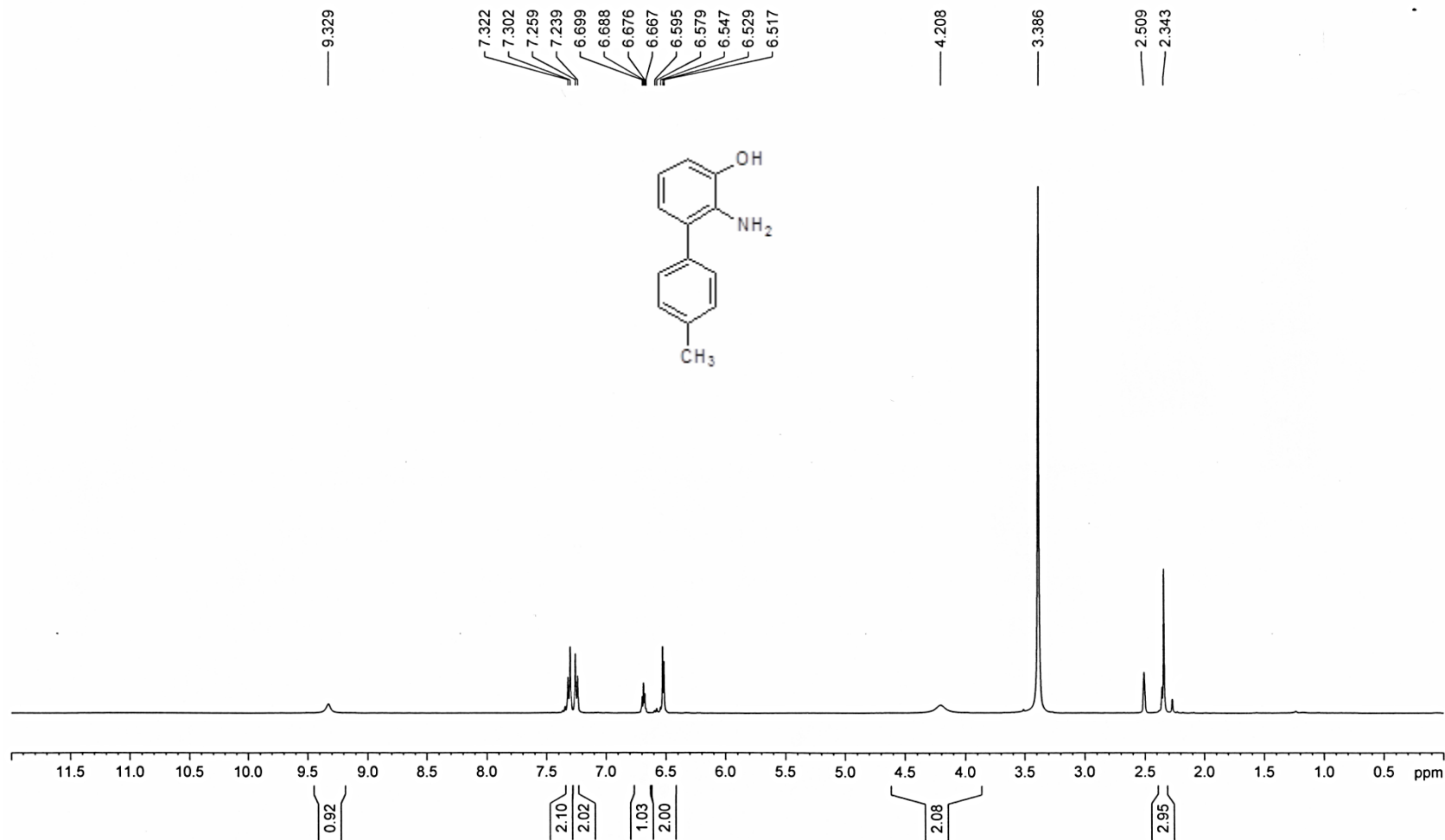
8.11.2019



^1H NMR of 2-Amino-4'-methyl-biphenyl-3-ol (5f)

^1H NMR NP-KS-4'-Me (5f) in DMSO- d_6

15.2.2020



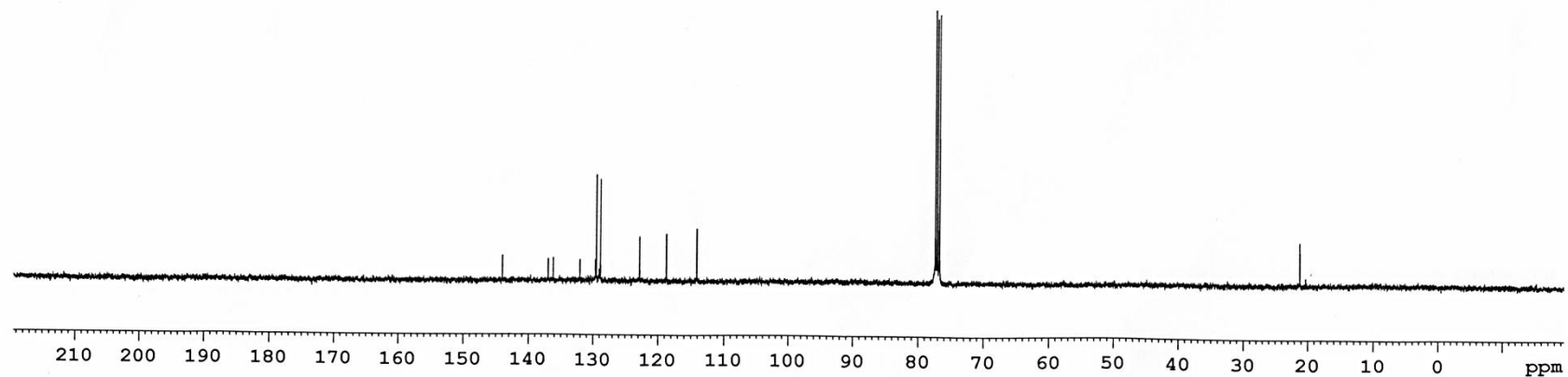
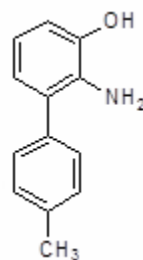
¹³C NMR of 2-Amino-4'-methyl-biphenyl-3-ol (5f)

¹³C of NP-KS-841 14.12.2019

143.99
136.98
136.21
132.06
129.66
129.51
128.89
122.83
118.71
114.10

77.37
77.05
76.73

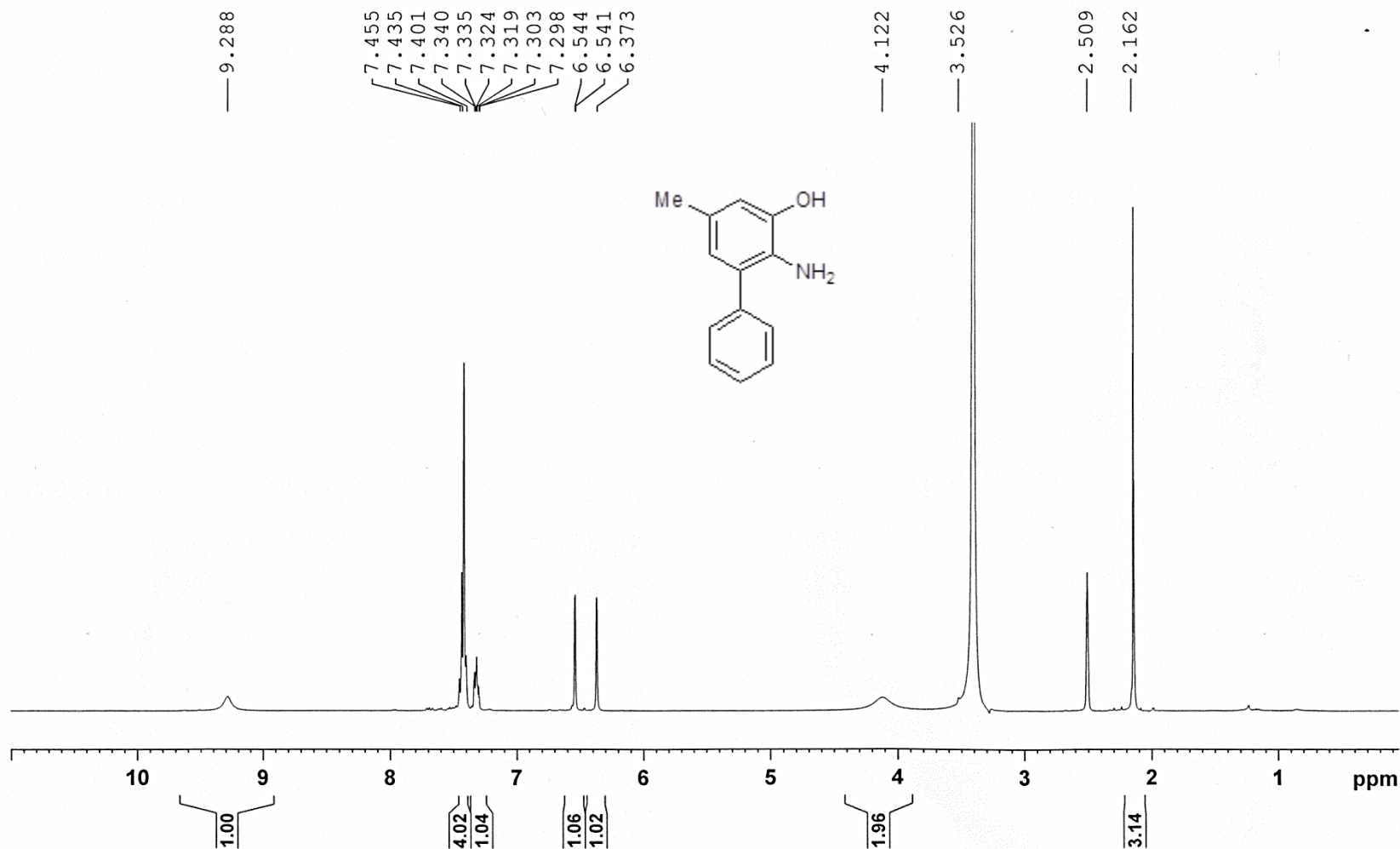
21.22



^1H NMR of 2-amino-5-methyl-biphenyl-3-ol (**5g**)

^1H NMR of NP-KS-5g in DMSO-d₆

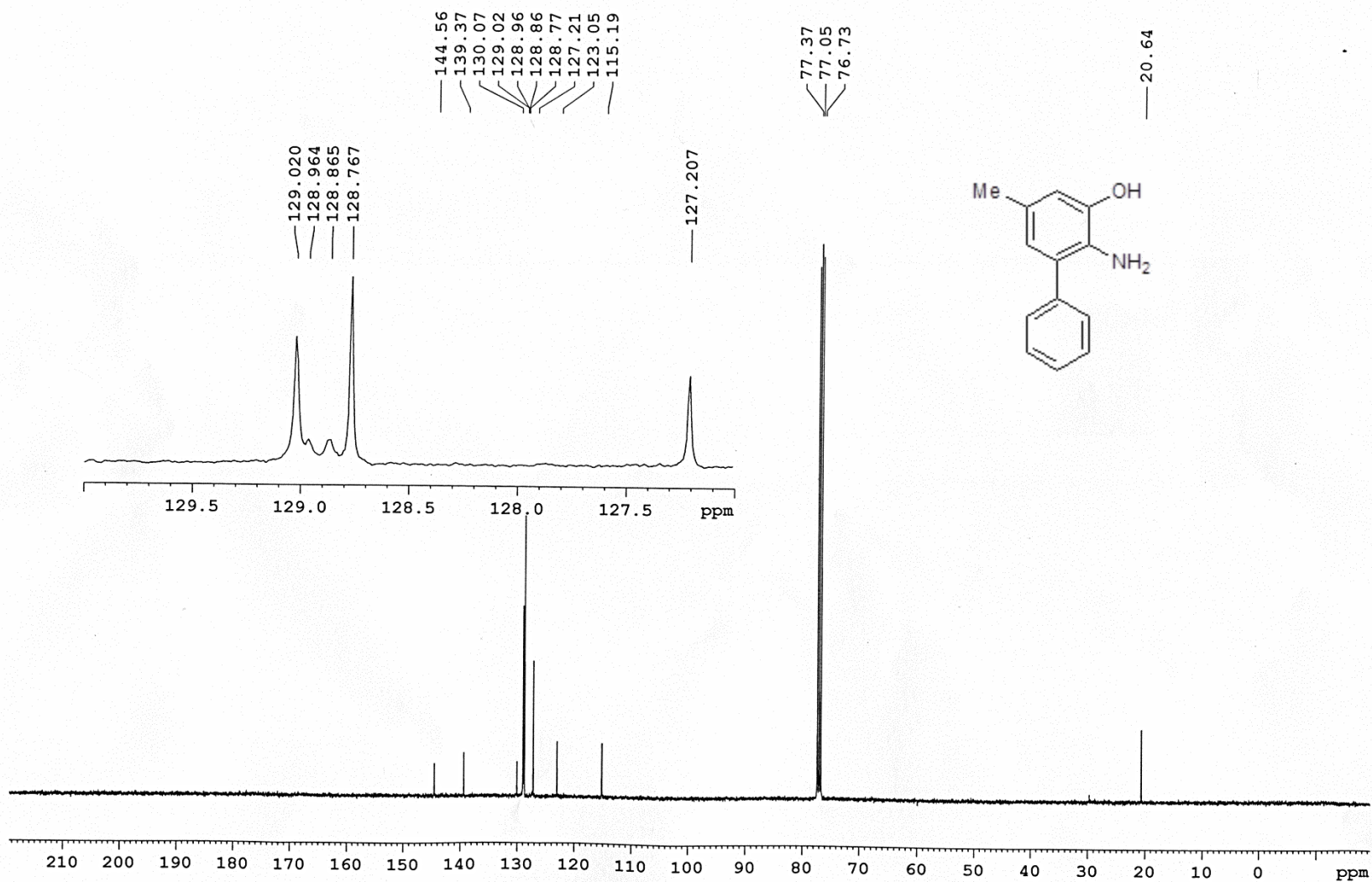
15.2.2020



^{13}C NMR of 2-Amino-5-methyl-biphenyl-3-ol (**5g**)

^{13}C of NP-KS-846

17.12.2019



Deuterium exchange experiment

¹H OF NP-KS-822 18.11.2019

